

10/529290

=> file registry

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DICTIONARY FILE UPDATES: 25 MAR 2008 HIGHEST RN 1010115-69-1

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=> file zcaplus

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FILE COVERS 1907 - 26 Mar 2008 VOL 148 ISS 13
FILE LAST UPDATED: 25 Mar 2008 (20080325/ED)

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This file contains CAS Registry Numbers for easy and accurate
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'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

=> d stat que L38

L35	17804	SEA	FILE=ZCAPLUS	ABB=ON	PLU=ON	TANAKA	S?/AU
L36	5183	SEA	FILE=ZCAPLUS	ABB=ON	PLU=ON	FUKUDA	K?/AU
L37	998	SEA	FILE=ZCAPLUS	ABB=ON	PLU=ON	ASADA	T?/AU
L38	1	SEA	FILE=ZCAPLUS	ABB=ON	PLU=ON	L35 AND L36 AND L37	

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=> d stat que L43

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L32      36798 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?PERFUM?/BI
L35      17804 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  TANAKA S?/AU
L36      5183  SEA FILE=ZCAPLUS ABB=ON  PLU=ON  FUKUDA K?/AU
L37      998   SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ASADA T?/AU
L39      41    SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L35 AND (L36 OR L37)
L43      11    SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L39 AND L32
```

=> file wpix

FILE 'WPIX' ENTERED AT 16:56:54 ON 26 MAR 2008

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FILE LAST UPDATED: 24 MAR 2008 <20080324/UP>

MOST RECENT THOMSON SCIENTIFIC UPDATE: 200820 <200820/DW>

DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

>>> IPC Reform backfile reclassification has been loaded to the end of November 2007. No update date (UP) has been created for the reclassified documents, but they can be identified by 20060101/UPIC and 20061231/UPIC, 20070601/UPIC, 20071001/UPIC and 20071130/UPIC. <<<

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http://www.stn-international.de/training_center/patents/stn_guide.pdf

FOR DETAILS OF THE PATENTS COVERED IN CURRENT UPDATES, SEE

<http://scientific.thomson.com/support/patents/coverage/latestupdates/>

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http://www.stn-international.com/archive/presentations/DWPIAnaVist2_0710.pdf

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>>> ECLA Codes and Current US National Classifications have been added - see NEWS and HELP CHANGE <<<

>>> HELP for European Patent Classifications see HELP ECLA, HELP ICO <<<

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http://www.stn-international.de/stndatabases/details/ico_0801.zip

http://www.stn-international.de/stndatabases/details/epc_0801.zip

Supplement of all changed ECLA items:

http://www.stn-international.de/stndatabases/details/ecla_0802s.zip <<<

'BIX' IS DEFAULT SEARCH FIELD FOR 'WPIX' FILE

=> s L43

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      17396 TANAKA S?/AU
      5776  FUKUDA K?/AU
      1486  ASADA T?/AU
      30920 ?PERFUM?/BI
L49      10 L39 AND L32
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=> dup rem L38 L39 L49

FILE 'ZCAPLUS' ENTERED AT 16:57:13 ON 26 MAR 2008

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PROCESSING COMPLETED FOR L38
PROCESSING COMPLETED FOR L39
PROCESSING COMPLETED FOR L49
L50 41 DUP REM L38 L39 L49 (11 DUPLICATES REMOVED)
ANSWERS '1-41' FROM FILE ZCAPLUS

=> dup rem L38 L43 L49
PROCESSING COMPLETED FOR L38
PROCESSING COMPLETED FOR L43
PROCESSING COMPLETED FOR L49
L51 11 DUP REM L38 L43 L49 (11 DUPLICATES REMOVED)
ANSWERS '1-11' FROM FILE ZCAPLUS

=> d ibib abs hitind hitstr L51 1-11

L51 ANSWER 1 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 1
ACCESSION NUMBER: 2007:618990 ZCAPLUS Full-text
DOCUMENT NUMBER: 147:30745
TITLE: Process for preparation of α,β -unsaturated
aldehydes via intramolecular condensation of aldehydes
in the presence of amines and proton acids.
INVENTOR(S): Ishida, Kosaku; Tanaka, Shigeyoshi; Asada, Takahiro
PATENT ASSIGNEE(S): Kao Corporation, Japan
SOURCE: PCT Int. Appl., 28pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2007063703	A1	20070607	WO 2006-JP322699	20061108
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
JP 2007153764	A	20070621	JP 2005-348121	20051201
PRIORITY APPLN. INFO.:			JP 2005-348121	A 20051201
OTHER SOURCE(S):	CASREACT 147:30745			

AB A process for preparation of α,β -unsatd. aldehydes comprises subjecting aldehydes to an intermol. condensation reaction in the presence of an amine and a protonic acid having 4-20 C atoms or a salt thereof. Thus, a mixture of campholenic aldehyde, piperidine, and stearic acid at 100° was treated with propionaldehyde over 6 h to give 95% 2-methyl-4-(2,2,3-trimethylcyclopent-3-en-1-yl)but-2-en-1-al of 60.6% purity. The latter was purified by distillation and reduced with LiAlH₄ in Et₂O to give 85% 2-methyl-4-(2,2,3-

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trimethylcyclopent-3-en-1-yl)but-2-en-1-ol. This had a sandalwood scent and was excellent as a perfume material.

CC 24-4 (Alicyclic Compounds)

Section cross-reference(s): 30, 62

ST aldehyde unsatd prepn; alc unsatd perfume; aldol condensation amine
protonic base

IT Perfumes

(unsatd. alcs.)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L51 ANSWER 2 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 2

ACCESSION NUMBER: 2004:292019 ZCAPLUS Full-text

DOCUMENT NUMBER: 140:321236

TITLE: Preparation of valerolactone compounds and perfume
composition

INVENTOR(S): Tanaka, Sakuya; Fukuda, Kazuyuki; Asada, Takahiro

PATENT ASSIGNEE(S): Kao Corporation, Japan

SOURCE: PCT Int. Appl., 65 pp.

CODEN: PIXXD2

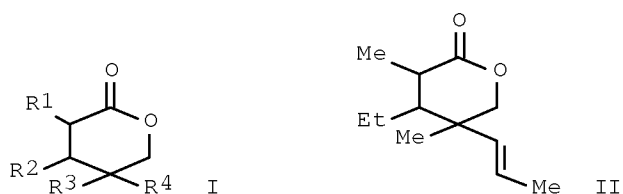
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004029033	A1	20040408	WO 2003-JP12341	20030926
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
JP 2004161746	A	20040610	JP 2003-323125	20030916
AU 2003272896	A1	20040419	AU 2003-272896	20030926
EP 1555261	A1	20050720	EP 2003-753957	20030926
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
CN 1684949	A	20051019	CN 2003-823085	20030926
IN 2005CN00483	A	20070824	IN 2005-CN483	20050324
US 2006258559	A1	20061116	US 2005-529290	20050325
IN 2007CN01476	A	20070928	IN 2007-CN1476	20070412
PRIORITY APPLN. INFO.:			JP 2002-282675	A 20020927
			JP 2002-308952	A 20021023
			JP 2003-323125	A 20030916
			WO 2003-JP12341	W 20030926
			IN 2005-CN483	A3 20050324
OTHER SOURCE(S):	MARPAT 140:321236			
GI				



AB Disclosed are a valerolactone compound represented by the formula (I) (wherein R1 and R2 each independently represents hydrogen, Me, or ethyl; R3 represents hydrogen or methyl; and R4 represents Pr, 1-propenyl, or phenyl; provided that not both of R1 and R2 are hydrogen), in particular, the valerolactone compound represented by the formula (II), and a process for producing that compound, and a perfume composition containing any of the valerolactone compds. Compds. I are useful as perfume or flavor compns. for household products, cosmetics, public health products, beverages, and foods such as detergents, fabric softeners, shampoos, body cleansers, milk flavors, milk coffee, or perfumes. Thus, Michael addition reaction of 2-pentenitrile with di-Me methylmalonate in the presence of NaOMe in methanol at 130° for 7 h and reduction of the resulting di-Me 2-methyl-2-[1-(cyanomethyl)propyl]malonate by LiBH₄ in THF at 30° for 3 h gave 3-(cyanomethyl)-2-methyl-2-hydroxymethyl-1-pentanol which underwent hydrolysis in aqueous NaOH solution at 97° for 2.5 h and acidification with 6 N aqueous HCl solution to give 4-ethyl-5-(hydroxymethyl)-5-methyl-tetrahydropyran-2-one (III). Oxidation of III by pyridinium dichromate in CH₂Cl₂ at room temperature for 17 h and Wittig reaction of the resulting 4-ethyl-5-formyl-5-methyltetrahydropyran-2-one with ethyltriphenylphosphonium bromide using PhLi in hexane/THF gave 4-ethyl-5-methyl-5-(cis-1-propenyl)tetrahydropyran-2-one which underwent cis-trans isomerization in the presence of thiophenol and 2,2'-bisazobutyronitrile at 80° for 2 h to give 4-ethyl-5-methyl-5-(trans-1-propenyl)tetrahydropyran-2-one.

IC ICM C07D309-30

ICS A61K007-46; C11B009-00; A23L001-226; A23L002-00

CC 27-13 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 17, 62

L51 ANSWER 3 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 3

ACCESSION NUMBER: 2000:765408 ZCAPLUS Full-text

DOCUMENT NUMBER: 133:321651

TITLE: Preparation of alkylcyclohexanones and their fragrance compositions

INVENTOR(S): Hashizume, Naomichio; Fukuda, Kazuyuki; Tanaka, Shigeyoshi; Koshino, Junji

PATENT ASSIGNEE(S): Kao Corp., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

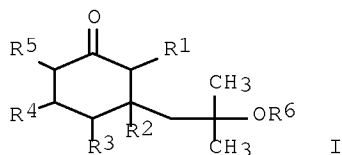
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 2000302722	A	20001031	JP 1999-115263	19990422
PRIORITY APPLN. INFO.:			JP 1999-115263	19990422

10/529290

OTHER SOURCE(S): MARPAT 133:321651
GI



AB Alkylcyclohexanones I (R1-R6 = H, Me, Et; the total number of C in R1-R6 is ≤3) are prepared 2-Methyl-1-propenylmagnesium bromide was treated with 2-cyclohexenone, and the condensation product was hydrogenated by NaBH4, methoxylated, and oxidized with pyridinium chlorochromate to give 10% I (R1-R5 = H, R6 = Me). The product had floral, fruity, and green odor.

IC ICM C07C049-517

ICS A61K007-46; C11B009-00

CC 24-5 (Alicyclic Compounds)

Section cross-reference(s): 62

IT Odor and Odorous substances

Perfumes

(preparation of alkylcyclohexanones for fragrance compns.)

L51 ANSWER 4 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 4

ACCESSION NUMBER: 2000:761945 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 133:321648

TITLE: Preparation of cyclohexanols and their fragrance compositions

INVENTOR(S): Hashizume, Naomichio; Fukuda, Kazuyuki; Tanaka, Shigeyoshi; Koshino, Junji

PATENT ASSIGNEE(S): Kao Corp., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

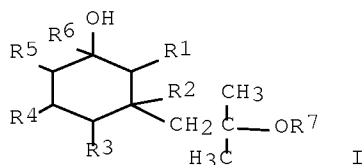
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 2000302713	A	20001031	JP 1999-115262	19990422
PRIORITY APPLN. INFO.:			JP 1999-115262	19990422
OTHER SOURCE(S):		MARPAT 133:321648		

GI



AB Cyclohexanols I (R1-R7 = H, Me, Et; the total number of C in R1-R7 is ≤3) are prepared 3-(2-Methylpropenyl)cyclohexanone was hydrogenated by NaBH4 at room temperature for 12 h in THF and the product was treated with MeOH and H2SO4 at -70° for 12 h to give 15% I (R1-R6 = H, R7 = Me). The product had floral, muguet, and sandalwood-like odor.

IC ICM C07C035-08
ICS C07C043-13; C11B009-00; C11D003-50; C11D009-44

CC 24-5 (Alicyclic Compounds)

IT Odor and Odorous substances
Perfumes
(preparation of cyclohexanols for fragrance compns.)

L51 ANSWER 5 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 5

ACCESSION NUMBER: 2000:765402 ZCAPLUS Full-text

DOCUMENT NUMBER: 133:321650

TITLE: Preparation of cyclohexylmethanols and their fragrance compositions

INVENTOR(S): Hashizume, Naomichio; Fukuda, Kazuyuki; Tanaka, Shigeyoshi; Koshino, Junji

PATENT ASSIGNEE(S): Kao Corp., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent

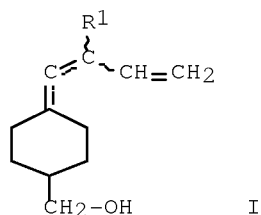
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 2000302712	A	20001031	JP 1999-110760	19990419
PRIORITY APPLN. INFO.:			JP 1999-110760	19990419
OTHER SOURCE(S):	MARPAT 133:321650			

GI



AB Cyclohexylmethanols I (R1 = H, Me; the broken line is an optional bond) are prepared Condensation of Me2CO with 4-hydroxymethylcyclohexanecarbaldehyde gave the corresponding α,β-unsatd. ketone, which was hydrogenated with NaBH4 and dehydrated to afford 19% I (R1 = H). The product had floral and grapefruit-like odor.

IC ICM C07C033-14

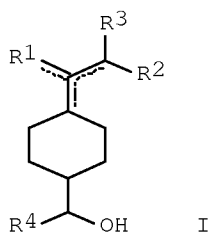
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ICS A61K007-46; C11B009-00; C11D003-50; C11D009-44
 CC 24-5 (Alicyclic Compounds)
 Section cross-reference(s): 62
 IT Odor and Odorous substances
 Perfumes
 (preparation of cyclohexylmethanols for fragrance compns.)

L51 ANSWER 6 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 6
 ACCESSION NUMBER: 2000:408806 ZCAPLUS Full-text
 DOCUMENT NUMBER: 133:30534
 TITLE: Preparation of cyclohexylalkanols as perfume raw material
 INVENTOR(S): Tanaka, Shigeyoshi; Yamamoto, Junko; Koshino, Junji; Fukuda, Kazuyuki; Toi, Naoshi
 PATENT ASSIGNEE(S): Kao Corp., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000169409	A	20000620	JP 1998-345611	19981204
JP 3756332	B2	20060315		
PRIORITY APPLN. INFO.:			JP 1998-345611	19981204
OTHER SOURCE(S):	MARPAT	133:30534		

GI



AB The title compds. (I; R1, R2, R3, R4 = H, Me, or Et and a total number of carbon atoms in R1-R4 is 2-3; a single line accompanied by a parallel dotted line appearing in three locations each represent a single or a double bond and one of these bonds represent a double bond.) are prepared These compds. possess floral fragrance and are useful as perfume components for toiletries. Thus, isopropyltriphenylphosphonium iodide was treated with potassium tert-butoxide in THF at room temperature for 1 h, and cooled in ice, followed by adding a solution of 4-(tetrahydropyran-2-ylloxymethyl)cyclohexanecarboxaldehyde (preparation given) in THF, and the resulting mixture was stirred at 25° for 4 h to give, after deprotection of tetrahydropyranyl group by p-MeC6H4SO3H in MeOH, title compound (II).

IC ICM C07C033-14
 ICS A61K007-46; C11B009-00
 CC 24-5 (Alicyclic Compounds)
 Section cross-reference(s): 62

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ST cyclohexylalkanol prepn perfume

IT Odor and Odorous substances

Perfumes

(preparation of cyclohexylalkanols as perfume raw material)

IT 273735-14-1P 273735-16-3P 273735-17-4P 273933-07-6P 273933-08-7P

RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of cyclohexylalkanols as perfume raw material)

IT 78-93-3, Methyl ethyl ketone, reactions 110-87-2, Dihydropyran
873-75-6, p-Bromobenzyl alcohol 4762-30-5, sec-Butyltriphenylphosphonium
iodide 5391-88-8 14350-50-6, n-Propyltriphenylphosphonium iodide
24470-78-8, Isopropyltriphenylphosphonium iodide 92385-32-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of cyclohexylalkanols as perfume raw material)

IT 17100-68-4P 273735-13-0P 273735-15-2P 273735-18-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of cyclohexylalkanols as perfume raw material)

L51 ANSWER 7 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 7

ACCESSION NUMBER: 1999:182540 ZCAPLUS Full-text

DOCUMENT NUMBER: 130:271888

TITLE: Cyclohexylalkanols and fragrance compositions
containing them

INVENTOR(S): Tanaka, Shigeyoshi; Yamamoto, Junko; Koshino, Junji;
Fukuda, Kazuyuki; Toi, Naoshi

PATENT ASSIGNEE(S): Kao Corp., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

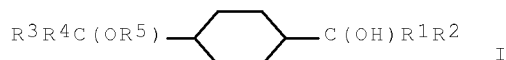
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 11071312	A	19990316	JP 1997-230792	19970827
JP 4027471	B2	20071226		
PRIORITY APPLN. INFO.:			JP 1997-230792	19970827
OTHER SOURCE(S):	MARPAT	130:271888		

GI



AB Fragrance compns., which show long-lasting fragrance, contain title compds. I (R¹-R⁴ = C₁-3 alkyl, H; R⁵ = C₁-3 alkyl). 4-Bromobenzyl alc. was etherified with MeI in THF in the presence of NaH, converted into Grignard reagent, treated with MeCHO in THF at room temperature for 12 h, and reduced by H in i-PrOH using Ru/C at 90° under 0.5 MPa for 3 days to give 38% I (R¹ = R⁵ = Me, R²-R⁴ = H), which showed woody, floral, and muguet-like fragrance for 4 days.

IC ICM C07C043-13

ICS C11B009-00

CC 62-5 (Essential Oils and Cosmetics)

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Section cross-reference(s): 24

IT Perfumes

(preparation of cyclohexylalkanols for fragrance compns.)

L51 ANSWER 8 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 8

ACCESSION NUMBER: 1999:107143 ZCAPLUS Full-text

DOCUMENT NUMBER: 130:213502

TITLE: Perfume compositions containing 4-alkoxymethylcyclohexylmethanols

INVENTOR(S): Tanaka, Shigeyoshi; Yamamoto, Junko; Koshino, Junji; Toi, Tadashi; Fukuda, Kazuyuki

PATENT ASSIGNEE(S): Kao Corp., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

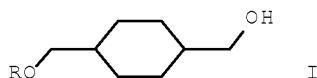
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 11035969	A	19990209	JP 1997-188069	19970714
JP 3833347	B2	20061011		
PRIORITY APPLN. INFO.:			JP 1997-188069	19970714
OTHER SOURCE(S):	MARPAT	130:213502		

GI



AB The compns. contain the title compds. I (R = C1-10 alkyl, C3-10 cycloalkyl, C2-10 alkenyl). The compns. have stable fragrance like lily of the valley. A floral fragrance for detergents was formulated from hexylcinnamic aldehyde 200, phenylethylalc. 200, rhodinol 200, citronellol 150, hydroxycitronellal 50, and I (R = Et) (preparation given) 200 parts.

IC ICM C11B009-00

ICS A61K007-00; A61K007-46; A61K007-50

CC 62-5 (Essential Oils and Cosmetics)

ST floral perfume alkoxymethylcyclohexylmethanol prepn; cyclohexylmethanol alkoxymethyl prepn floral perfume

IT Cosmetics

Detergents

Perfumes

(preparation of 4-alkoxymethylcyclohexylmethanols having fragrance like

lily

of the valley and perfume compns. containing them)

IT 33424-86-1P, 4-Allyloxymethylcyclohexylmethanol 98955-27-2P,

4-Methoxymethylcyclohexylmethanol 220331-53-3P, 4-

Ethoxymethylcyclohexylmethanol 220331-54-4P, 4-

Isopropoxymethylcyclohexylmethanol

RL: BUU (Biological use, unclassified); PNU (Preparation, unclassified);

TEM (Technical or engineered material use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 4-alkoxymethylcyclohexylmethanols having fragrance like

10/529290

lily

of the valley and perfume compns. containing them)

IT 74-88-4, Methyl iodide, reactions 74-96-4, Ethyl bromide 75-30-9,
2-Iodopropane 105-08-8, 1,4-Dimethylolcyclohexane 556-56-9, Allyl
iodide

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of 4-alkoxymethylcyclohexylmethanols having fragrance like

lily

of the valley and perfume compns. containing them)

L51 ANSWER 9 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 9

ACCESSION NUMBER: 1998:485420 ZCAPLUS Full-text

DOCUMENT NUMBER: 129:179988

TITLE: 2,2-Dimethyl-3-alkoxypropanols and fragrance
compositions containing these

INVENTOR(S): Tanaka, Shigeyoshi; Koshino, Junji; Fukuda,
Kazuyuki; Toi, Naoshi

PATENT ASSIGNEE(S): Kao Corp., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
JP 10195010	A	19980728	JP 1997-577	19970107
PRIORITY APPLN. INFO.:			JP 1997-577	19970107

OTHER SOURCE(S): MARPAT 129:179988

AB Fragrance compns. contain HOCH2CMe2CH2OCH2R (R = C3-6 branched alkyl). Acid-
catalyzed cyclization of isobutyraldehyde with 2,2-dimethyl-1,3- propanediol
to give a 1,3-dioxane derivative followed by reduction with diisobutylaluminum
hydride gave 2,2-dimethyl-3-(2-methylpropyloxy)-1- propanol, which showed
floral odor.

IC ICM C07C043-13

ICS C11B009-00

CC 62-5 (Essential Oils and Cosmetics)

Section cross-reference(s): 23

ST methylalkoxypropanol prepn perfume; propanol methylalkoxy prepn
perfume; fragrance dimethylalkoxypropanol prepn

IT Perfumes

(preparation of 2,2-dimethyl-3-alkoxypropanols for fragrance compns.)

L51 ANSWER 10 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 10

ACCESSION NUMBER: 1997:416661 ZCAPLUS Full-text

DOCUMENT NUMBER: 127:55670

TITLE: Perfumes containing 4-(2-methoxyphenyl)-2-methyl-2-
butanol

INVENTOR(S): Tanaka, Shigeyoshi; Etsuno, Junji; Fukuda,
Kazuyuki; Toi, Sunao

PATENT ASSIGNEE(S): Kao Corp., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

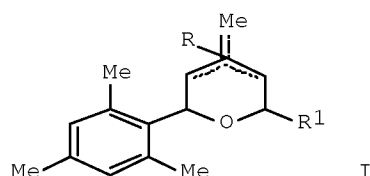
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
------------	------	------	-----------------	------

 JP 09111281 A 19970428 JP 1995-270893 19951019
 JP 3462319 B2 20031105
 PRIORITY APPLN. INFO.: JP 1995-270893 19951019
 AB The title compound with flowery scent is prepared and formulated with other
 aromatic compds. for cosmetics and perfumes.
 IC ICM C11B009-00
 ICS C11D003-50
 CC 62-5 (Essential Oils and Cosmetics)
 ST methoxyphenylmethylbutanol prepn perfume
 IT Perfumes
 (perfumes containing 4-(2-methoxyphenyl)-2-methyl-2-butanol)
 IT 56052-48-3P
 RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL
 (Biological study); PREP (Preparation); USES (Uses)
 (perfumes containing 4-(2-methoxyphenyl)-2-methyl-2-butanol)
 IT 105-36-2, Ethyl bromoacetate 135-02-4, o-Anisaldehyde
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (perfumes containing 4-(2-methoxyphenyl)-2-methyl-2-butanol)
 IT 70200-18-9P 70311-27-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (perfumes containing 4-(2-methoxyphenyl)-2-methyl-2-butanol)

L51 ANSWER 11 OF 11 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2006:142819 ZCAPLUS Full-text
 DOCUMENT NUMBER: 144:232917
 TITLE: Preparation of novel pyrans and perfume compositions
 containing them
 INVENTOR(S): Asada, Takahiro; Tanaka, Shigeyoshi
 PATENT ASSIGNEE(S): Kao Corp., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2006045111	A	20060216	JP 2004-228018	20040804
PRIORITY APPLN. INFO.:			JP 2004-228018	20040804
OTHER SOURCE(S):	MARPAT 144:232917			

GI



AB Pyrans I (R = H, OH; when R = H, then 1 of the broken lines may be double bond; when R = OH; all the broken lines = single bonds; R1 = H, Me) are

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prepared by cyclization of 2,4,6-trimethylbenzaldehyde (II) with H₂C:CM₂CH₂CHR₁OH (R₁ = same as above) in the presence of acid catalysts. Thus, II was treated with isoprenol and p-toluenesulfonic acid at 100°C for 3 h to give I (R = R₁ = H; 1 of the broken lines is double bond) and I (R = R₁ = H; all the broken lines = single bonds), which possessed herbal odor and sweet odor, resp.

CC 27-13 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 62
ST trimethylphenyl pyran prepn perfume; trimethylbenzaldehyde cyclization
isoprenol toluenesulfonic acid catalyst
IT Cyclocondensation reaction catalysts
Perfumes
(preparation of (trimethylphenyl)pyrans for perfume compns.)
IT Acids, uses
RL: CAT (Catalyst use); USES (Uses)
(preparation of (trimethylphenyl)pyrans for perfume compns.)
IT 104-15-4, p-Toluenesulfonic acid, uses
RL: CAT (Catalyst use); USES (Uses)
(preparation of (trimethylphenyl)pyrans for perfume compns.)
IT 876132-59-1P
RL: COS (Cosmetic use); RCT (Reactant); SPN (Synthetic preparation); BIOL
(Biological study); PREP (Preparation); RACT (Reactant or reagent); USES
(Uses)
(preparation of (trimethylphenyl)pyrans for perfume compns.)
IT 876132-58-0P 876132-60-4P 876132-61-5P 876132-62-6P 876132-63-7P
876132-64-8P
RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological
study); PREP (Preparation); USES (Uses)
(preparation of (trimethylphenyl)pyrans for perfume compns.)
IT 487-68-3, 2,4,6-Trimethylbenzaldehyde 763-32-6, Isoprenol 2004-67-3,
4-Methyl-4-penten-2-ol
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of (trimethylphenyl)pyrans for perfume compns.)

=> file marpat

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FILE CONTENT: 1961-PRESENT VOL 148 ISS 11 (20080321/ED)

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(COVERAGE TO THESE DATES IS NOT COMPLETE):

US 2008032917 07 FEB 2008
DE 102006035202 31 JAN 2008
EP 1882693 30 JAN 2008
JP 2008024674 07 FEB 2008
WO 2008021152 21 FEB 2008
GB 2439172 19 DEC 2007
FR 2904316 01 FEB 2008
RU 2316552 10 FEB 2008
CA 2593150 06 JAN 2008

Expanded G-group definition display now available.

10/529290

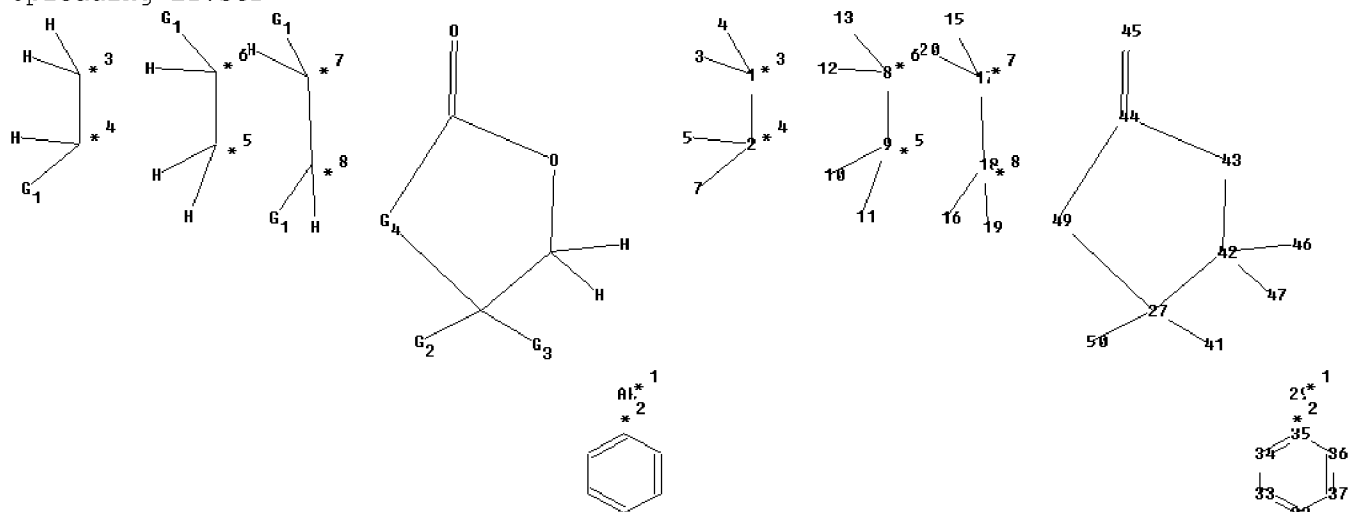
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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:

Uploading L1.str



chain nodes :

3 4 5 7 10 11 12 13 15 16 19 20 29 41 45 46 47 50

ring nodes :

1 2 8 9 17 18 27 32 33 34 35 36 37 42 43 44 49

chain bonds :

1-3 1-4 2-5 2-7 8-12 8-13 9-10 9-11 15-17 16-18 17-20 18-19 27-41 27-50

42-46 42-47 44-45

ring bonds :

1-2 8-9 17-18 27-49 27-42 32-33 32-37 33-34 34-35 35-36 36-37 42-43 43-44

44-49

exact/norm bonds :

1-3 1-4 2-5 2-7 8-12 8-13 9-10 9-11 15-17 16-18 17-20 18-19 27-41 27-50

42-46 42-47 44-45

exact bonds :

1-2 8-9 17-18 27-49 27-42 42-43 43-44 44-49

normalized bonds :

32-33 32-37 33-34 34-35 35-36 36-37

G1:CH3,Et

G2:CH3,H

G3:[*1],[*2]

G4:[*3-*4],[*5-*6],[*7-*8]

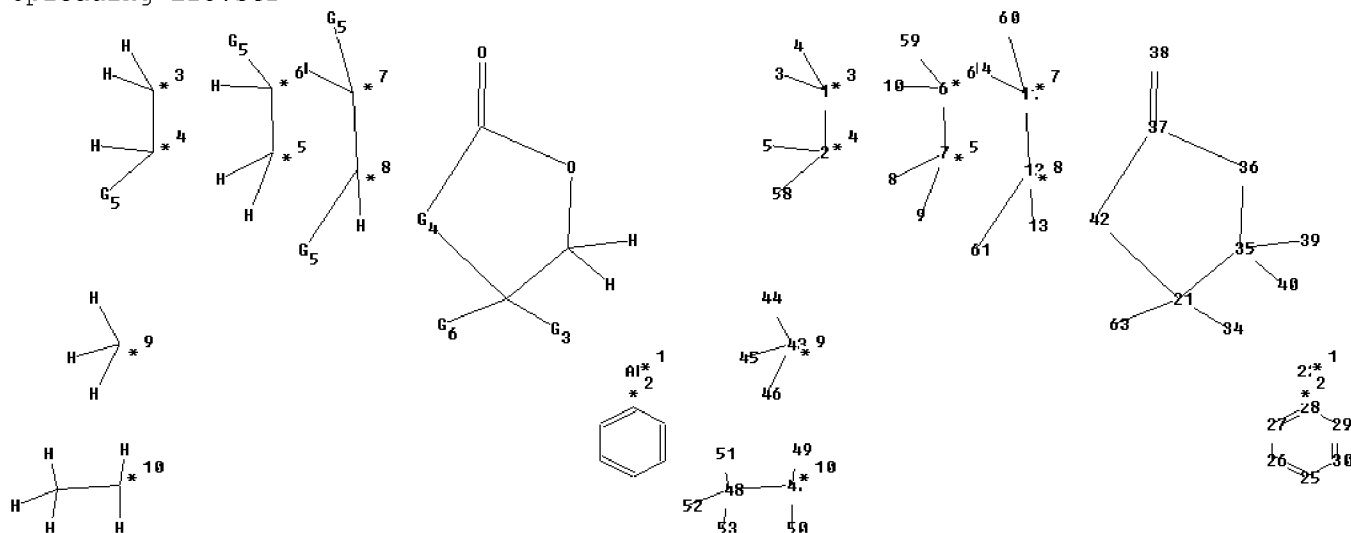
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Connectivity :
29:1 E exact RC ring/chain
Match level :
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11:CLASS
12:CLASS 13:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:CLASS 20:CLASS
27:Atom 29:CLASS
32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 41:CLASS 42:Atom 43:Atom
44:Atom 45:CLASS
46:CLASS 47:CLASS 49:Atom 50:CLASS
Element Count :
Node 29: Limited
C,C3

L24 96 SEA FILE=MARPAT SSS FUL L1
L25 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
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chain nodes :
3 4 5 8 9 10 13 14 22 34 38 39 40 43 44 45 46 47 48 49 50 51
52 53 58 59 60 61 63
ring nodes :
1 2 6 7 11 12 21 25 26 27 28 29 30 35 36 37 42
chain bonds :
1-3 1-4 2-5 2-58 6-10 6-59 7-8 7-9 11-14 11-60 12-13 12-61 21-34 21-63
35-39 35-40 37-38 43-44 43-45 43-46 47-48 47-49 47-50 48-51 48-52 48-53
ring bonds :
1-2 6-7 11-12 21-42 21-35 25-26 25-30 26-27 27-28 28-29 29-30 35-36 36-
37
37-42
exact/norm bonds :

10/529290

1-3 1-4 2-5 2-58 6-10 6-59 7-8 7-9 11-14 11-60 12-13 12-61 21-34 21-63
35-39 35-40 37-38 43-44 43-45 43-46 47-48 47-49 47-50 48-51 48-52 48-53
exact bonds :
1-2 6-7 11-12 21-42 21-35 35-36 36-37 37-42
normalized bonds :
25-26 25-30 26-27 27-28 28-29 29-30

G3:[*1],[*2]

G4:[*3-*4],[*5-*6],[*7-*8]

G5:[*9],[*10]

G6:H,[*9]

Connectivity :

22:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:CLASS 4:CLASS 5:CLASS 6:Atom 7:Atom 8:CLASS 9:CLASS
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11:Atom 12:Atom 13:CLASS 14:CLASS 21:Atom 22:Atom 25:Atom 26:Atom 27:Atom
28:Atom 29:Atom

30:Atom 34:CLASS 35:Atom 36:Atom 37:Atom 38:Atom 39:CLASS 40:CLASS 42:Atom
43:Atom

44:CLASS 45:CLASS 46:CLASS 47:Atom 48:Atom 49:CLASS 50:CLASS 51:CLASS

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Element Count :

Node 22: Limited

C,C3

L27 17 SEA FILE=MARPAT SUB=L24 SSS FUL L25
L47 1 SEA FILE=MARPAT ABB=ON PLU=ON ("140:321236"/AN OR "2004:29201
9"/AN)
L48 1 SEA FILE=MARPAT ABB=ON PLU=ON L47 AND L27

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L48 ANSWER 1 OF 1 MARPAT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 140:321236 MARPAT Full-text

TITLE: Preparation of valerolactone compounds and perfume
composition

INVENTOR(S): Tanaka, Sakuya; Fukuda, Kazuyuki; Asada, Takahiro

PATENT ASSIGNEE(S): Kao Corporation, Japan

SOURCE: PCT Int. Appl., 65 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

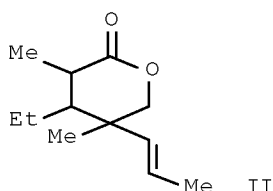
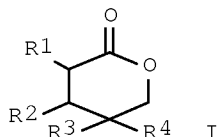
FAMILY ACC. NUM. COUNT: 1

10/529290

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2004029033	A1	20040408	WO 2003-JP12341	20030926
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
JP 2004161746	A	20040610	JP 2003-323125	20030916
AU 2003272896	A1	20040419	AU 2003-272896	20030926
EP 1555261	A1	20050720	EP 2003-753957	20030926
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
CN 1684949	A	20051019	CN 2003-823085	20030926
IN 2005CN00483	A	20070824	IN 2005-CN483	20050324
US 2006258559	A1	20061116	US 2005-529290	20050325
IN 2007CN01476	A	20070928	IN 2007-CN1476	20070412
PRIORITY APPLN. INFO.:			JP 2002-282675	20020927
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			WO 2003-JP12341	20030926
			IN 2005-CN483	20050324

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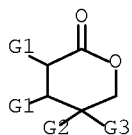


AB Disclosed are a valerolactone compound represented by the formula (I) (wherein R1 and R2 each independently represents hydrogen, Me, or ethyl; R3 represents hydrogen or methyl; and R4 represents Pr, 1-propenyl, or phenyl; provided that not both of R1 and R2 are hydrogen), in particular, the valerolactone compound represented by the formula (II), and a process for producing that compound, and a perfume composition containing any of the valerolactone compds. Compds. I are useful as perfume or flavor compns. for household products, cosmetics, public health products, beverages, and foods such as detergents, fabric softeners, shampoos, body cleansers, milk flavors, milk coffee, or perfumes. Thus, Michael addition reaction of 2-pentenitrile with di-Me methylmalonate in the presence of NaOMe in methanol at 130° for 7 h and reduction of the resulting di-Me 2-methyl-2-[1-(cyanomethyl)propyl]malonate by LiBH₄ in THF at 30° for 3 h gave 3-(cyanomethyl)-2-methyl-2-hydroxymethyl-1-pentanol which

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underwent hydrolysis in aqueous NaOH solution at 97° for 2.5 h and acidification with 6 N aqueous HCl solution to give 4-ethyl-5-(hydroxymethyl)-5-methyl-tetrahydropyran-2-one (III). Oxidation of III by pyridinium dichromate in CH₂Cl₂ at room temperature for 17 h and Wittig reaction of the resulting 4-ethyl-5-formyl-5-methyltetrahydropyran-2-one with ethyltriphenylphosphonium bromide using PhLi in hexane/THF gave 4-ethyl-5-methyl-5-(cis-1-propenyl)tetrahydropyran-2-one which underwent cis-trans isomerization in the presence of thiophenol and 2,2'-bisazobutyronitrile at 80° for 2 h to give 4-ethyl-5-methyl-5-(trans-1-propenyl)tetrahydropyran-2-one.

MSTR 1



G1 = Me
G3 = Pr-n

Patent location:

claim 1

10/529290

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DICTIONARY FILE UPDATES: 25 MAR 2008 HIGHEST RN 1010115-69-1

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FILE LAST UPDATED: 25 Mar 2008 (20080325/ED)

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=> d stat que L14

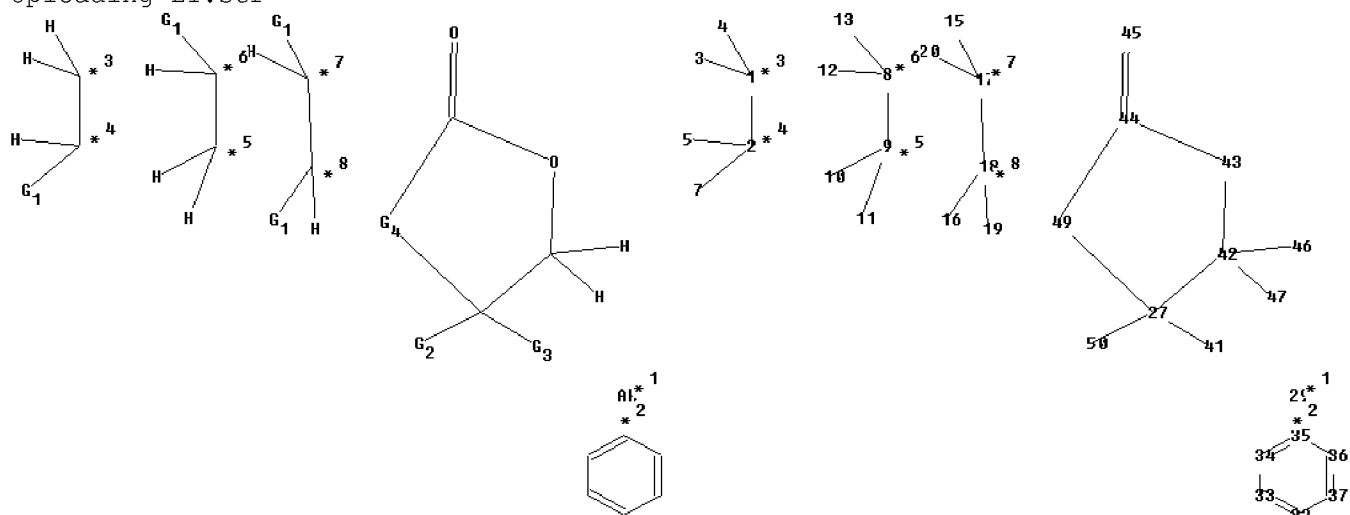
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Structure attributes must be viewed using STN Express query preparation:

10/529290

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ring nodes :
1 2 8 9 17 18 27 32 33 34 35 36 37 42 43 44 49
chain bonds :
1-3 1-4 2-5 2-7 8-12 8-13 9-10 9-11 15-17 16-18 17-20 18-19 27-41 27-
50
42-46 42-47 44-45
ring bonds :
1-2 8-9 17-18 27-49 27-42 32-33 32-37 33-34 34-35 35-36 36-37 42-43 43-
44
44-49
exact/norm bonds :
1-3 1-4 2-5 2-7 8-12 8-13 9-10 9-11 15-17 16-18 17-20 18-19 27-41 27-
50
42-46 42-47 44-45
exact bonds :
1-2 8-9 17-18 27-49 27-42 42-43 43-44 44-49
normalized bonds :
32-33 32-37 33-34 34-35 35-36 36-37

```

G1:CH3,Et

G2:CH3,H

G3:[*1],[*2]

G4:[*3-*4],[*5-*6],[*7-*8]

Connectivity :

29:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:CLASS 4:CLASS 5:CLASS 7:CLASS 8:Atom 9:Atom 10:CLASS
11:CLASS

12:CLASS 13:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:CLASS 20:CLASS

27:Atom 29:CLASS

32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 41:CLASS 42:Atom 43:Atom

44:Atom 45:CLASS

46:CLASS 47:CLASS 49:Atom 50:CLASS

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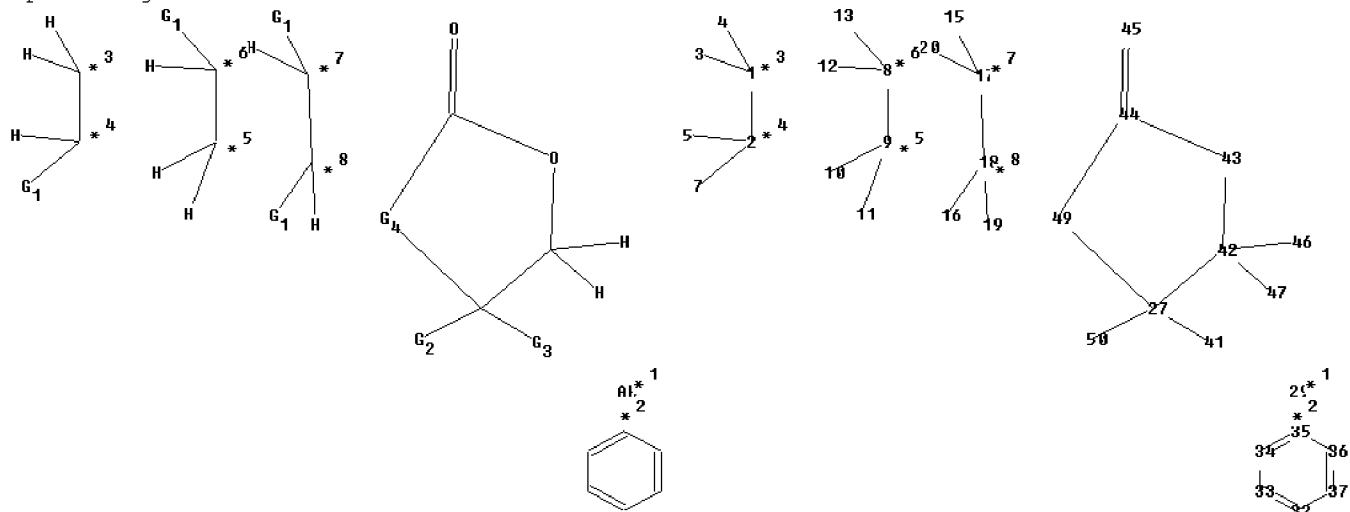
Element Count :
Node 29: Limited
C,C3

L9 16 SEA FILE=REGISTRY SSS FUL L1
L14 7 SEA FILE=ZCAPLUS ABB=ON PLU=ON L9

=> d stat que L15
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
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chain nodes :
3 4 5 7 10 11 12 13 15 16 19 20 29 41 45 46 47 50
ring nodes :
1 2 8 9 17 18 27 32 33 34 35 36 37 42 43 44 49
chain bonds :
1-3 1-4 2-5 2-7 8-12 8-13 9-10 9-11 15-17 16-18 17-20 18-19 27-41 27-50
42-46 42-47 44-45
ring bonds :
1-2 8-9 17-18 27-49 27-42 32-33 32-37 33-34 34-35 35-36 36-37 42-43 43-44
44-49
exact/norm bonds :
1-3 1-4 2-5 2-7 8-12 8-13 9-10 9-11 15-17 16-18 17-20 18-19 27-41 27-50
42-46 42-47 44-45
exact bonds :
1-2 8-9 17-18 27-49 27-42 42-43 43-44 44-49
normalized bonds :
32-33 32-37 33-34 34-35 35-36 36-37

10/529290

G1:CH3,Et

G2:CH3,H

G3:[*1],[*2]

G4:[*3-*4],[*5-*6],[*7-*8]

Connectivity :

29:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:CLASS 4:CLASS 5:CLASS 7:CLASS 8:Atom 9:Atom 10:CLASS

11:CLASS

12:CLASS 13:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:CLASS 20:CLASS

27:Atom 29:CLASS

32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 41:CLASS 42:Atom 43:Atom

44:Atom 45:CLASS

46:CLASS 47:CLASS 49:Atom 50:CLASS

Element Count :

Node 29: Limited

C,C3

```
L6          32 SEA FILE=REGISTRY ABB=ON  PLU=ON  (107898-54-4/BI OR 123-38-6/B
I OR 126-98-7/BI OR 13284-42-9/BI OR 1530-32-1/BI OR 23727-15-3
/B I OR 28219-60-5/BI OR 28219-61-6/BI OR 609-02-9/BI OR
623-36-9/BI OR 65113-99-7/BI OR 677326-31-7/BI OR 677326-32-8/B
I OR 677326-33-9/BI OR 677326-34-0/BI OR 677326-35-1/BI OR
677326-36-2/BI OR 677326-37-3/BI OR 677326-38-4/BI OR 677326-39
-5/BI OR 677326-40-8/BI OR 677326-41-9/BI OR 677326-42-0/BI OR
677326-43-1/BI OR 677326-44-2/BI OR 677326-45-3/BI OR 677326-46
-4/BI OR 677763-76-7/BI OR 677763-77-8/BI OR 67801-20-1/BI OR
72089-08-8/BI OR 93-53-8/BI)
L7          14 SEA FILE=REGISTRY ABB=ON  PLU=ON  L6 AND OC5/ES
L9          16 SEA FILE=REGISTRY SSS FUL L1
L10         9 SEA FILE=REGISTRY ABB=ON  PLU=ON  L9 AND L7
L11         5 SEA FILE=REGISTRY ABB=ON  PLU=ON  L7 NOT L10
L12        6097 SEA FILE=REGISTRY ABB=ON  PLU=ON  C10H18O2/MF
L13         1 SEA FILE=REGISTRY ABB=ON  PLU=ON  L11 AND L12
L14         7 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L9
L15         1 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L13 AND L14
```

=> d stat que L16

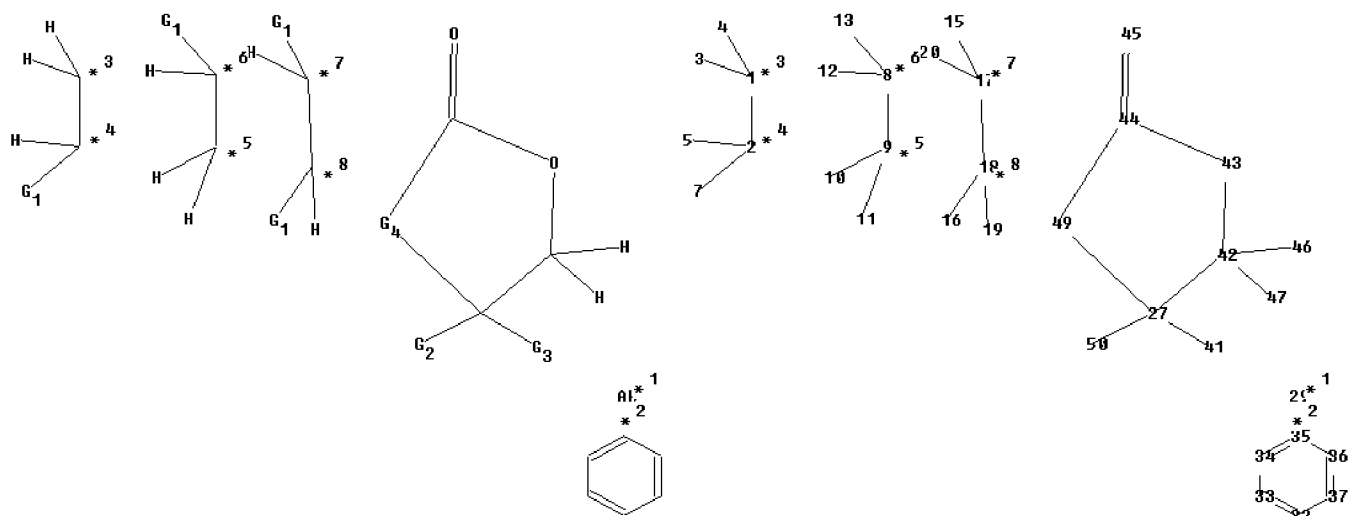
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:

Uploading L1.str

10/529290



chain nodes :

3 4 5 7 10 11 12 13 15 16 19 20 29 41 45 46 47 50

ring nodes :

1 2 8 9 17 18 27 32 33 34 35 36 37 42 43 44 49

chain bonds :

1-3 1-4 2-5 2-7 8-12 8-13 9-10 9-11 15-17 16-18 17-20 18-19 27-41 27-50

42-46 42-47 44-45

ring bonds :

1-2 8-9 17-18 27-49 27-42 32-33 32-37 33-34 34-35 35-36 36-37 42-43 43-44

44-49

exact/norm bonds :

1-3 1-4 2-5 2-7 8-12 8-13 9-10 9-11 15-17 16-18 17-20 18-19 27-41 27-50

42-46 42-47 44-45

exact bonds :

1-2 8-9 17-18 27-49 27-42 42-43 43-44 44-49

normalized bonds :

32-33 32-37 33-34 34-35 35-36 36-37

G1:CH3,Et

G2:CH3,H

G3:[*1],[*2]

G4:[*3-*4],[*5-*6],[*7-*8]

Connectivity :

29:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:CLASS 4:CLASS 5:CLASS 7:CLASS 8:Atom 9:Atom 10:CLASS

11:CLASS

12:CLASS 13:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:CLASS 20:CLASS

27:Atom 29:CLASS

32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 41:CLASS 42:Atom 43:Atom

44:Atom 45:CLASS

46:CLASS 47:CLASS 49:Atom 50:CLASS

Element Count :

10/529290

Node 29: Limited
C,C3

L6 32 SEA FILE=REGISTRY ABB=ON PLU=ON (107898-54-4/BI OR 123-38-6/B
I OR 126-98-7/BI OR 13284-42-9/BI OR 1530-32-1/BI OR 23727-15-3
/BI OR 28219-60-5/BI OR 28219-61-6/BI OR 609-02-9/BI OR
623-36-9/BI OR 65113-99-7/BI OR 677326-31-7/BI OR 677326-32-8/B
I OR 677326-33-9/BI OR 677326-34-0/BI OR 677326-35-1/BI OR
677326-36-2/BI OR 677326-37-3/BI OR 677326-38-4/BI OR 677326-39
-5/BI OR 677326-40-8/BI OR 677326-41-9/BI OR 677326-42-0/BI OR
677326-43-1/BI OR 677326-44-2/BI OR 677326-45-3/BI OR 677326-46
-4/BI OR 677763-76-7/BI OR 677763-77-8/BI OR 67801-20-1/BI OR
72089-08-8/BI OR 93-53-8/BI)
L9 16 SEA FILE=REGISTRY SSS FUL L1
L14 7 SEA FILE=ZCAPLUS ABB=ON PLU=ON L9
L16 2 SEA FILE=ZCAPLUS ABB=ON PLU=ON L6 AND L14

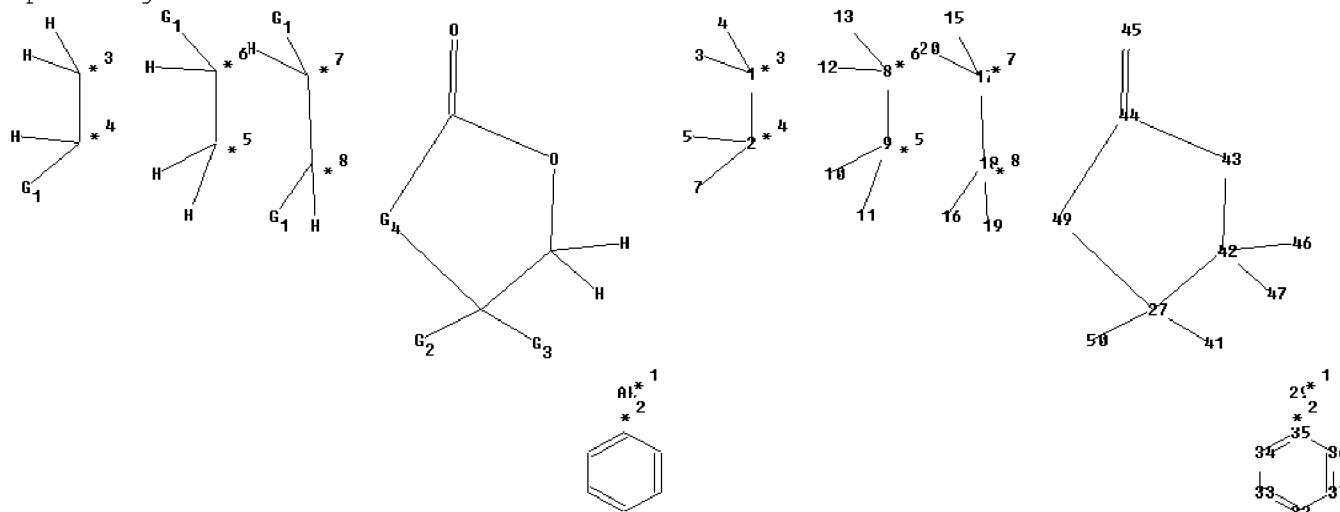
=> d stat que L33

L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:

Uploading L1.str



chain nodes :

3 4 5 7 10 11 12 13 15 16 19 20 29 41 45 46 47 50

ring nodes :

1 2 8 9 17 18 27 32 33 34 35 36 37 42 43 44 49

chain bonds :

1-3 1-4 2-5 2-7 8-12 8-13 9-10 9-11 15-17 16-18 17-20 18-19 27-41 27-50

42-46 42-47 44-45

ring bonds :

1-2 8-9 17-18 27-49 27-42 32-33 32-37 33-34 34-35 35-36 36-37 42-43 43-44

10/529290

44-49

exact/norm bonds :

1-3 1-4 2-5 2-7 8-12 8-13 9-10 9-11 15-17 16-18 17-20 18-19 27-41 27-50

42-46 42-47 44-45

exact bonds :

1-2 8-9 17-18 27-49 27-42 42-43 43-44 44-49

normalized bonds :

32-33 32-37 33-34 34-35 35-36 36-37

G1:CH3,Et

G2:CH3,H

G3:[*1],[*2]

G4:[*3-*4],[*5-*6],[*7-*8]

Connectivity :

29:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:CLASS 4:CLASS 5:CLASS 7:CLASS 8:Atom 9:Atom 10:CLASS 11:CLASS

12:CLASS 13:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:CLASS 20:CLASS

27:Atom 29:CLASS

32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 41:CLASS 42:Atom 43:Atom

44:Atom 45:CLASS

46:CLASS 47:CLASS 49:Atom 50:CLASS

Element Count :

Node 29: Limited

C,C3

L9 16 SEA FILE=REGISTRY SSS FUL L1

L33 1 SEA FILE=ZCAPLUS ABB=ON PLU=ON L9 (L) COS/RL

=> d stat que L34

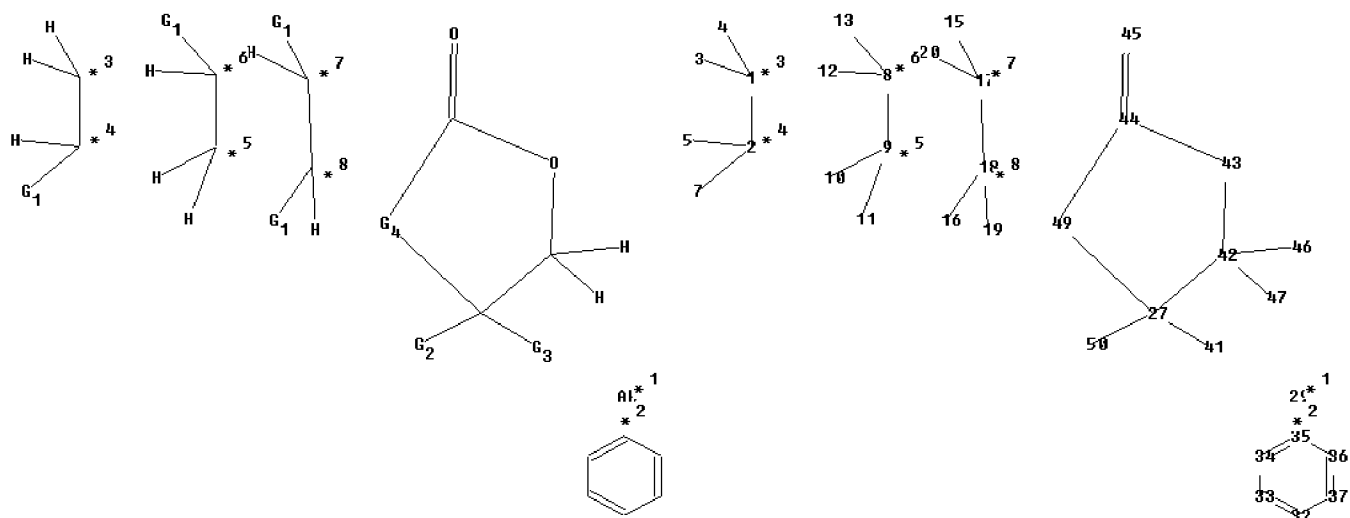
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:

Uploading L1.str

10/529290



chain nodes :

3 4 5 7 10 11 12 13 15 16 19 20 29 41 45 46 47 50

ring nodes :

1 2 8 9 17 18 27 32 33 34 35 36 37 42 43 44 49

chain bonds :

1-3 1-4 2-5 2-7 8-12 8-13 9-10 9-11 15-17 16-18 17-20 18-19 27-41 27-50

42-46 42-47 44-45

ring bonds :

1-2 8-9 17-18 27-49 27-42 32-33 32-37 33-34 34-35 35-36 36-37 42-43 43-44

44-49

exact/norm bonds :

1-3 1-4 2-5 2-7 8-12 8-13 9-10 9-11 15-17 16-18 17-20 18-19 27-41 27-50

42-46 42-47 44-45

exact bonds :

1-2 8-9 17-18 27-49 27-42 42-43 43-44 44-49

normalized bonds :

32-33 32-37 33-34 34-35 35-36 36-37

G1:CH3,Et

G2:CH3,H

G3:[*1],[*2]

G4:[*3-*4],[*5-*6],[*7-*8]

Connectivity :

29:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:CLASS 4:CLASS 5:CLASS 7:CLASS 8:Atom 9:Atom 10:CLASS

11:CLASS

12:CLASS 13:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:CLASS 20:CLASS

27:Atom 29:CLASS

32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 41:CLASS 42:Atom 43:Atom

44:Atom 45:CLASS

46:CLASS 47:CLASS 49:Atom 50:CLASS

Element Count :

10/529290

Node 29: Limited
C,C3

```
L9          16 SEA FILE=REGISTRY SSS FUL L1
L14         7 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L9
L31        89969 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  COSME?/BI
L32        36798 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  ?PERFUM?/BI
L34         1 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L14 AND (L31 OR L32)
```

```
=> s L14-L16 or L33-L34
L52         7 (L14 OR L15 OR L16) OR (L33 OR L34)
```

```
=> s L52 not L38,L43
L53         6 L52 NOT (L38 OR L43)
```

=> file beilstein

FILE 'BEILSTEIN' ENTERED AT 16:59:48 ON 26 MAR 2008
COPYRIGHT (c) 2008 Beilstein-Institut zur Foerderung der Chemischen Wissenschaften
licensed to Beilstein GmbH and MDL Information Systems GmbH

FILE LAST UPDATED ON January 3, 2008

FILE COVERS 1771 TO 2007.

*** FILE CONTAINS 10.119,480 SUBSTANCES ***

>>>PLEASE NOTE: Reaction Data and substance data are stored in
separate documents and can not be searched together in one query.
Reaction data for BEILSTEIN compounds may be displayed
immediately with the display codes PRE (preparations) and REA
(reactions). A substance answer set retrieved after the search
for a chemical name, a compounds with available reaction
information by combining with PRE/FA, REA/FA or more generally
with RX/FA. The BEILSTEIN Registry Number (BRN) is the link
between a BEILSTEIN compound and belonging reactions. For mo
detailed reaction searches BRNs can be searched as reaction
partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

```
*****
* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. *
* FOR PRICE INFORMATION SEE HELP COST *
*****
```

>>> Price change as of January 1st, 2008: Connect Time and Structure
Search fees re-introduced. See NEWS and HELP COST <<<

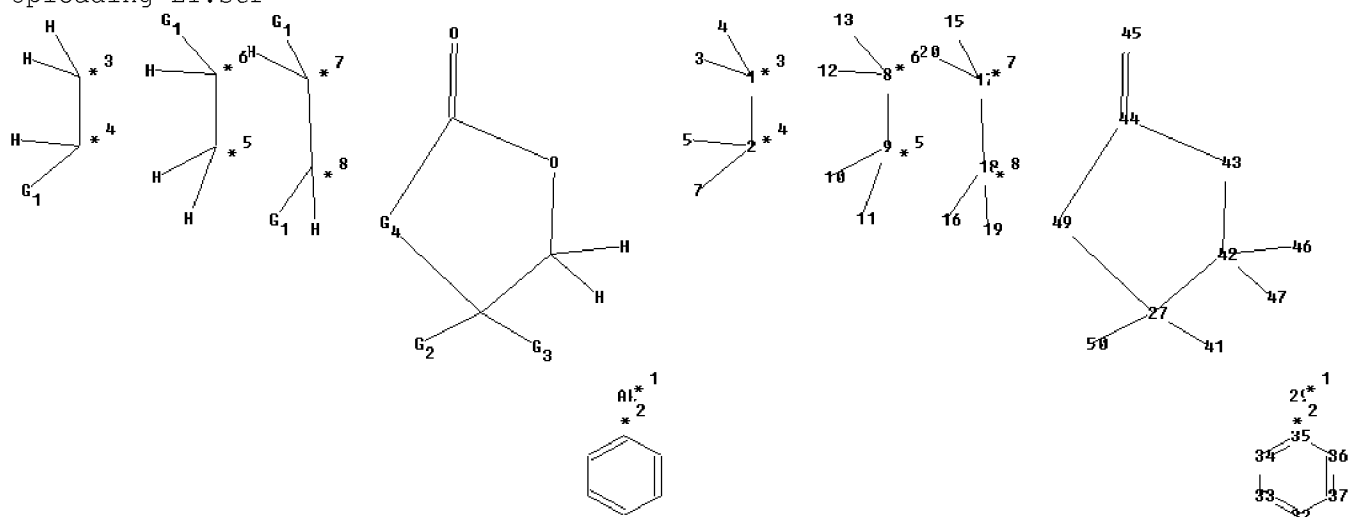
```
=> d stat que L21
L1          STR
```

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

10/529290

Structure attributes must be viewed using STN Express query preparation:

Uploading L1.str



chain nodes :

3 4 5 7 10 11 12 13 15 16 19 20 29 41 45 46 47 50

ring nodes :

1 2 8 9 17 18 27 32 33 34 35 36 37 42 43 44 49

chain bonds :

1-3 1-4 2-5 2-7 8-12 8-13 9-10 9-11 15-17 16-18 17-20 18-19 27-41 27-50

42-46 42-47 44-45

ring bonds :

1-2 8-9 17-18 27-49 27-42 32-33 32-37 33-34 34-35 35-36 36-37 42-43 43-44

44-49

exact/norm bonds :

1-3 1-4 2-5 2-7 8-12 8-13 9-10 9-11 15-17 16-18 17-20 18-19 27-41 27-50

42-46 42-47 44-45

exact bonds :

1-2 8-9 17-18 27-49 27-42 42-43 43-44 44-49

normalized bonds :

32-33 32-37 33-34 34-35 35-36 36-37

G1:CH3,Et

G2:CH3,H

G3:[*1],[*2]

G4:[*3-*4],[*5-*6],[*7-*8]

Connectivity :

29:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:CLASS 4:CLASS 5:CLASS 7:CLASS 8:Atom 9:Atom 10:CLASS

11:CLASS

12:CLASS 13:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:CLASS 20:CLASS

27:Atom 29:CLASS

32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 41:CLASS 42:Atom 43:Atom

10/529290

44:Atom 45:CLASS
46:CLASS 47:CLASS 49:Atom 50:CLASS
Element Count :
Node 29: Limited
C,C3

L19 SCR 1338
L21 4 SEA FILE=BEILSTEIN SSS FUL L1 AND L19

100.0% PROCESSED 145067 ITERATIONS 4 ANSWERS
SEARCH TIME: 00.01.35

=> file marpat
FILE 'MARPAT' ENTERED AT 17:00:01 ON 26 MAR 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE CONTENT: 1961-PRESENT VOL 148 ISS 11 (20080321/ED)

SOME MARPAT RECORDS ARE DERIVED FROM INPI DATA FOR 1961-1987

MOST RECENT CITATIONS FOR PATENTS FROM MAJOR ISSUING AGENCIES
(COVERAGE TO THESE DATES IS NOT COMPLETE):

US	2008032917	07 FEB 2008
DE	102006035202	31 JAN 2008
EP	1882693	30 JAN 2008
JP	2008024674	07 FEB 2008
WO	2008021152	21 FEB 2008
GB	2439172	19 DEC 2007
FR	2904316	01 FEB 2008
RU	2316552	10 FEB 2008
CA	2593150	06 JAN 2008

Expanded G-group definition display now available.

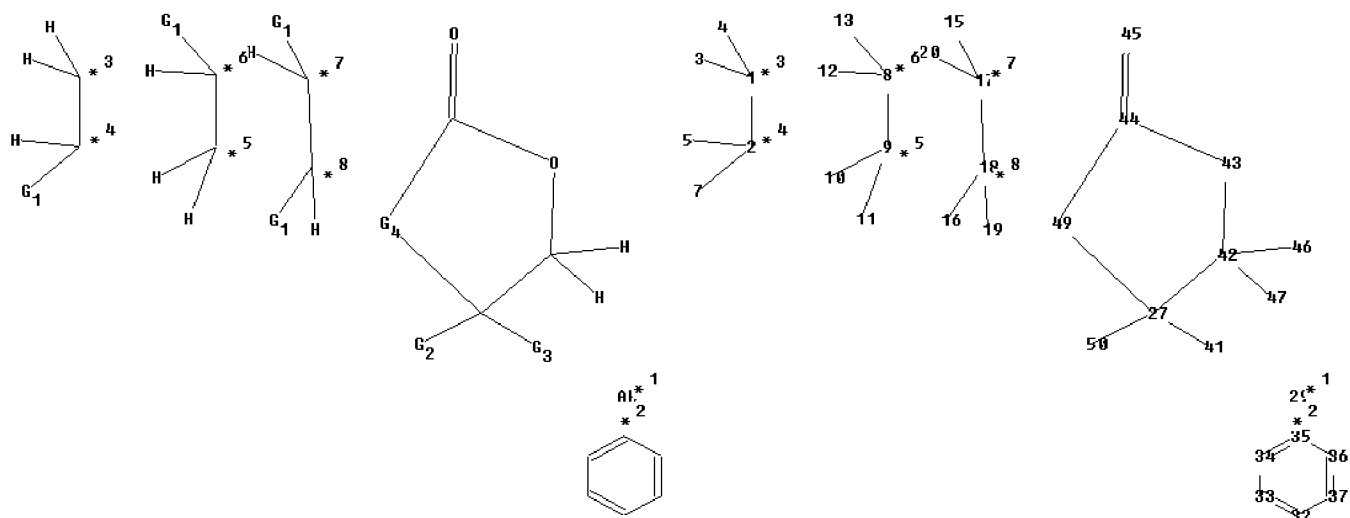
Effective December 15th the iteration and answer limits in MARPAT have increased from 100,000 to 200,000 for both on-line and batch searches. For more information on MARPAT search limits, type HELP SLIMITS at an arrow prompt.

=> d stat que L27
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
Uploading L1.str

10/529290



chain nodes :

3 4 5 7 10 11 12 13 15 16 19 20 29 41 45 46 47 50

ring nodes :

1 2 8 9 17 18 27 32 33 34 35 36 37 42 43 44 49

chain bonds :

1-3 1-4 2-5 2-7 8-12 8-13 9-10 9-11 15-17 16-18 17-20 18-19 27-41 27-50

42-46 42-47 44-45

ring bonds :

1-2 8-9 17-18 27-49 27-42 32-33 32-37 33-34 34-35 35-36 36-37 42-43 43-44

44-49

exact/norm bonds :

1-3 1-4 2-5 2-7 8-12 8-13 9-10 9-11 15-17 16-18 17-20 18-19 27-41 27-50

42-46 42-47 44-45

exact bonds :

1-2 8-9 17-18 27-49 27-42 42-43 43-44 44-49

normalized bonds :

32-33 32-37 33-34 34-35 35-36 36-37

G1:CH3,Et

G2:CH3,H

G3:[*1],[*2]

G4:[*3-*4],[*5-*6],[*7-*8]

Connectivity :

29:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:CLASS 4:CLASS 5:CLASS 7:CLASS 8:Atom 9:Atom 10:CLASS 11:CLASS

12:CLASS 13:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:CLASS 20:CLASS 27:Atom 29:CLASS

32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 41:CLASS 42:Atom 43:Atom 44:Atom 45:CLASS

46:CLASS 47:CLASS 49:Atom 50:CLASS

Element Count :

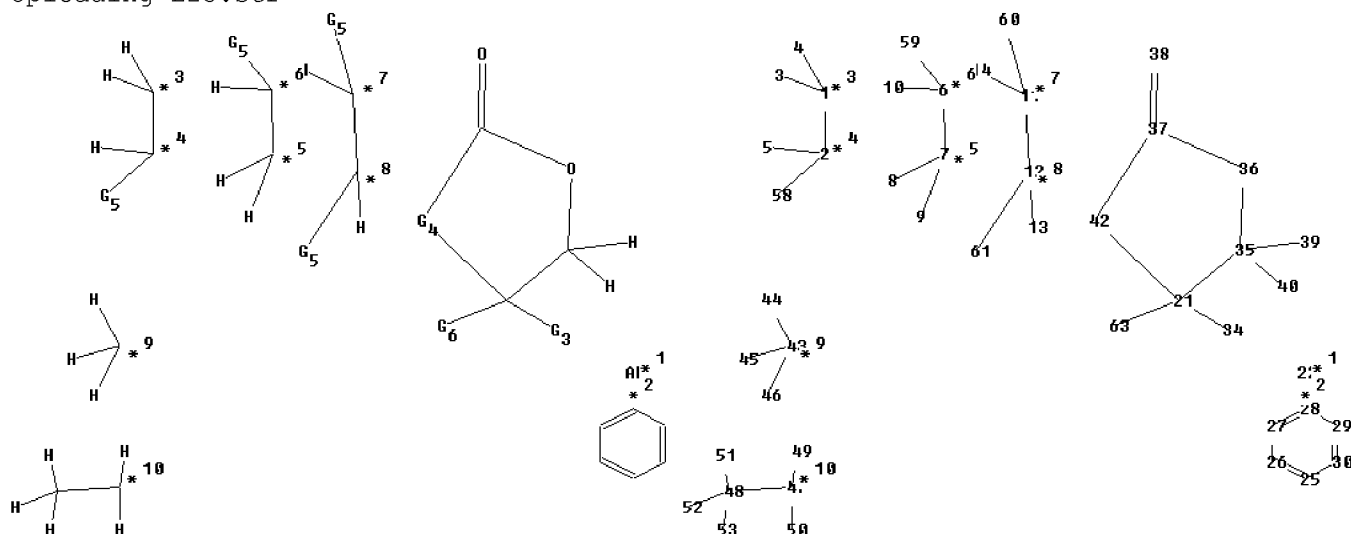
10/529290

Node 29: Limited
C,C3

L24 96 SEA FILE=MARPAT SSS FUL L1
L25 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
Uploading L25.str



chain nodes :

3 4 5 8 9 10 13 14 22 34 38 39 40 43 44 45 46 47 48 49 50 51
52 53 58 59 60 61 63

ring nodes :

1 2 6 7 11 12 21 25 26 27 28 29 30 35 36 37 42

chain bonds :

1-3 1-4 2-5 2-58 6-10 6-59 7-8 7-9 11-14 11-60 12-13 12-61 21-34 21-63
35-39 35-40 37-38 43-44 43-45 43-46 47-48 47-49 47-50 48-51 48-52 48-53

ring bonds :

1-2 6-7 11-12 21-42 21-35 25-26 25-30 26-27 27-28 28-29 29-30 35-36 36-37

37-42

exact/norm bonds :

1-3 1-4 2-5 2-58 6-10 6-59 7-8 7-9 11-14 11-60 12-13 12-61 21-34 21-63
35-39 35-40 37-38 43-44 43-45 43-46 47-48 47-49 47-50 48-51 48-52 48-53

exact bonds :

1-2 6-7 11-12 21-42 21-35 35-36 36-37 37-42

normalized bonds :

25-26 25-30 26-27 27-28 28-29 29-30

G3:[*1],[*2]

G4:[*3-*4],[*5-*6],[*7-*8]

10/529290

G5:[*9],[*10]

G6:H,[*9]

Connectivity :

22:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:CLASS 4:CLASS 5:CLASS 6:Atom 7:Atom 8:CLASS 9:CLASS
10:CLASS

11:Atom 12:Atom 13:CLASS 14:CLASS 21:Atom 22:Atom 25:Atom 26:Atom 27:Atom
28:Atom 29:Atom

30:Atom 34:CLASS 35:Atom 36:Atom 37:Atom 38:Atom 39:CLASS 40:CLASS 42:Atom
43:Atom

44:CLASS 45:CLASS 46:CLASS 47:Atom 48:Atom 49:CLASS 50:CLASS 51:CLASS

52:CLASS 53:CLASS

58:CLASS 59:CLASS 60:CLASS 61:CLASS 63:CLASS

Element Count :

Node 22: Limited

C,C3

L27 17 SEA FILE=MARPAT SUB=L24 SSS FUL L25

100.0% PROCESSED 91 ITERATIONS

17 ANSWERS

SEARCH TIME: 00.00.01

=> s l27 not L48

L54 16 L27 NOT L48

=> dup rem L53 L21 L54

DUPLICATE IS NOT AVAILABLE IN 'BEILSTEIN'.

ANSWERS FROM THESE FILES WILL BE CONSIDERED UNIQUE

FILE 'ZCAPLUS' ENTERED AT 17:00:26 ON 26 MAR 2008

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE 'BEILSTEIN' ENTERED AT 17:00:26 ON 26 MAR 2008

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FILE 'MARPAT' ENTERED AT 17:00:26 ON 26 MAR 2008

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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PROCESSING COMPLETED FOR L53

PROCESSING COMPLETED FOR L21

PROCESSING COMPLETED FOR L54

L55 26 DUP REM L53 L21 L54 (0 DUPLICATES REMOVED)

ANSWERS '1-6' FROM FILE ZCAPLUS

ANSWERS '7-10' FROM FILE BEILSTEIN

ANSWERS '11-26' FROM FILE MARPAT

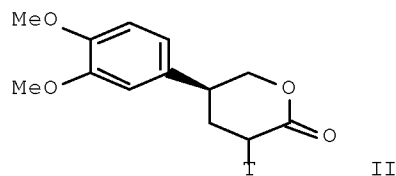
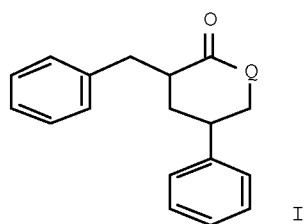
=> d ibib abs hitind hitstr L55 1-6; d ide allref L55 7-10; d ibib abs qhit L55 11-

L55 ANSWER 1 OF 26 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2003:777384 ZCAPLUS Full-text
 DOCUMENT NUMBER: 139:292150
 TITLE: preparation of lactams and lactones as
 antiinflammatories
 INVENTOR(S): Shen, Yaping; Burgoyne, David L.; Lauener, Ronald W.;
 Zhou, Yuanlin; Rebstein, Patrick J.; Abraham, Samuel
 D. M.
 PATENT ASSIGNEE(S): Inflazyme Pharmaceuticals Ltd., Can.
 SOURCE: U.S. Pat. Appl. Publ., 88 pp., Cont.-in-part of U.S.
 Ser. No. 81,993.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003186943	A1	20031002	US 2002-263336	20021001
US 6770658	B2	20040803		
WO 2000014083	A1	20000316	WO 1999-CA819	19990909
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,				
CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL,				
IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD,				
MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK,				
SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK,				
ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG,				
CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6458829	B1	20021001	US 2001-786949	20010511
CA 2500675	A1	20040415	CA 2003-2500675	20030930
WO 2004031149	A1	20040415	WO 2003-CA1506	20030930
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CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE,				
GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,				
LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ,				
OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,				
TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,				
KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,				
FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,				
BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003271478	A1	20040423	AU 2003-271478	20030930
EP 1551805	A1	20050713	EP 2003-753187	20030930
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IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006508069	T	20060309	JP 2004-540421	20030930
MX 2005PA03547	A	20050701	MX 2005-PA3547	20050401
PRIORITY APPLN. INFO.:			US 1998-99637P	P 19980909
			US 1999-121507P	P 19990223
			US 1999-149517P	P 19990817
			US 1999-393445	B1 19990908
			WO 1999-CA819	W 19990909
			US 2000-527699	B1 20000316
			US 2001-786949	A2 20010511
			US 2002-81993	A2 20020222
			US 2002-263336	A 20021001

OTHER SOURCE(S):
GI

MARPAT 139:292150



AB Title compds., e.g. [I; Q = multivalent atom other than C; each substitutable position may be substituted by W, R⁷W_n; W = NH₂, CONH₂, COOH, CN, CHO, OCHO, X, OH, NO₂, SH, COX, NHR₈, NR₈R₈, CONHR₈, CONR₈R₈, COOR₈, COR₈, OCOR₈, OR₈, BH₂, BHR₈, BR₈R₈, BO₂H₂, BO₂R₈R₈, PH₂, PHR₈, PR₈R₈, POR₈, PO₂R₈, PO₃R₈, SR₈; SOR₈, SO₂R₈, SONH₂, SONHR₈, SONR₈R₈, SO₂NH₂, SO₂NHR₈, SO₂NR₈R₈; R⁷ = hydrocarbyl, halocarbyl, hydrohalocarbyl wherein n of the H or halo atoms of R⁷ are substituted by W; R₈ = hydrocarbyl, halocarbyl, hydrohalocarbyl; n = 0-5; X = Br, Cl, F, iodo], were prepared Thus, n-BuLi was added to a solution of diisopropylamine in THF at -78 °; the mixture was stirred at -78° for 1 h, then HMPA was added, followed by a solution of (II; T = H) in THF. After 1 h, a solution of 4-(cyclopentyloxy)-3-methoxybenzyl bromide in THF was added to the reaction, and the resulting mixture was stirred at -78° for an addnl. 4 h to give II; T = 4-(cyclopentyloxy)-3-methoxybenzyl. The latter in a murine tail skin allograft transplantation model gave 100% allograft survival at 9 days post-transplant.

IC ICM A61K031-675

ICS A61K031-445; C07D211-40

INCL 514089000; 514317000; 546022000; 546216000

CC 27-16 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 1

IT	261357-66-8P	261357-73-7P	261357-79-3P	261357-86-2P	261357-98-6P
	261358-04-7P	261358-05-8P	261358-07-0P	261358-09-2P	261358-12-7P
	261358-14-9P	261358-15-0P	261358-16-1P	261358-21-8P	
	261358-22-9P	261358-23-0P	261358-35-4P	261358-40-1P	261358-42-3P
	261358-44-5P	261358-46-7P	261358-48-9P	261358-50-3P	261358-51-4P
	261358-52-5P	261358-53-6P	261358-54-7P	261358-55-8P	261358-56-9P
	261358-58-1P	261358-60-5P	261358-61-6P	261358-62-7P	261358-63-8P
	261358-64-9P	261358-65-0P	261358-66-1P	261358-67-2P	261358-68-3P
	261358-69-4P	261358-70-7P	261358-71-8P	261358-72-9P	261358-73-0P
	261358-74-1P	261358-75-2P	261358-76-3P	261358-77-4P	261358-78-5P
	261358-79-6P	261358-80-9P	261358-81-0P	261358-82-1P	261358-83-2P
	261358-84-3P	261358-85-4P	261358-86-5P	261358-87-6P	261358-88-7P
	261358-89-8P	261358-90-1P	261358-91-2P	261358-92-3P	261358-93-4P
	261358-94-5P	261358-95-6P	261358-96-7P	261358-97-8P	261358-98-9P
	261358-99-0P	608141-85-1P			

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of lactams and lactones as antiinflammatories)

IT 261358-15-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

10/529290

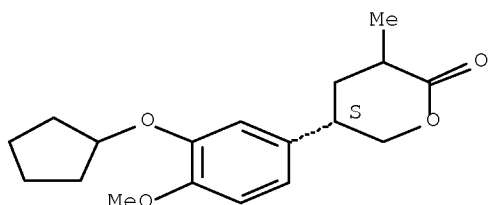
(Uses)

(preparation of lactams and lactones as antiinflammatories)

RN 261358-15-0 ZCAPLUS

CN 2H-Pyran-2-one, 5-[3-(cyclopentyloxy)-4-methoxyphenyl]tetrahydro-3-methyl-, (5S)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L55 ANSWER 2 OF 26 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:790729 ZCAPLUS Full-text

DOCUMENT NUMBER: 138:24849

TITLE: Synthesis of a Diels-Alder precursor for the Elisabethin A skeleton

AUTHOR(S): Heckrodt, Thilo J.; Mulzer, Johann

CORPORATE SOURCE: Institut für Organische Chemie der Universität Wien, Vienna, 1090, Austria

SOURCE: Synthesis (2002), (13), 1857-1866

CODEN: SYNTBF; ISSN: 0039-7881

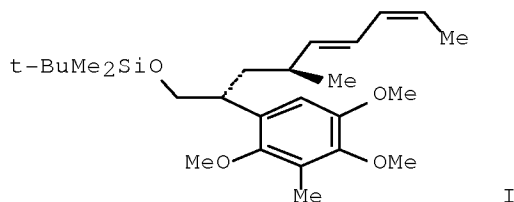
PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:24849

GI



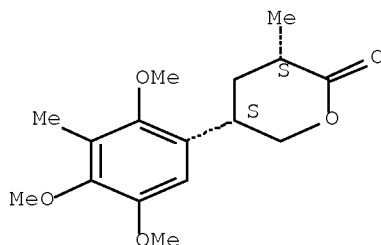
AB A synthesis of a precursor, I, for the elisabethin A skeleton is reported. Containing a masked quinone and a (E,Z)-diene subunit, it has the required elements for the envisaged intramol. Diels-Alder reaction to form the tricyclic system of elisabethin A. Starting from methylresorcinol, the sequence involves the preparation of an arylacetic acid, which was α -alkylated by a chiral building block. Subsequent HWE reaction and cis-selective Wittig olefination furnished the diene with the desired geometry.

CC 30-20 (Terpenes and Terpenoids)

10/529290

IT 19676-67-6P 212051-35-9P 478303-35-4P 478303-44-5P
 478303-53-6P 478303-54-7P 478303-55-8P 478303-61-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of a Diels-Alder precursor for the elisabethin A skeleton from
 methylresorcinol via α -alkylation of an arylacetic acid by a
 chiral building block, Horner-Wadsworth Emmons and cis-selective Wittig
 reactions)
 IT 478303-53-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of a Diels-Alder precursor for the elisabethin A skeleton from
 methylresorcinol via α -alkylation of an arylacetic acid by a
 chiral building block, Horner-Wadsworth Emmons and cis-selective Wittig
 reactions)
 RN 478303-53-6 ZCAPLUS
 CN 2H-Pyran-2-one, tetrahydro-3-methyl-5-(2,4,5-trimethoxy-3-methylphenyl)-,
 (3S,5S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



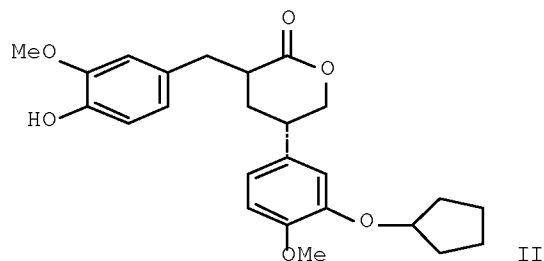
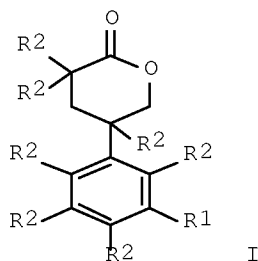
REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L55 ANSWER 3 OF 26 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2000:175807 ZCAPLUS Full-text
 DOCUMENT NUMBER: 132:222442
 TITLE: Preparation of substituted γ -phenyl- δ -
 lactones and analogs as antiinflammatory agents
 INVENTOR(S): Shen, Yaping; Burgoyne, David L.; Lauener, Ronald W.;
 Zhou, Yuanlin; Rebstein, Patrick J.; Abraham, Samuel
 D. M.
 PATENT ASSIGNEE(S): Inflazyme Pharmaceuticals Ltd., Can.
 SOURCE: PCT Int. Appl., 210 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000014083	A1	20000316	WO 1999-CA819	19990909
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK,				

ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG,
 CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

CA 2343732	A1	20000316	CA 1999-2343732	19990909
AU 9955009	A	20000327	AU 1999-55009	19990909
AU 757052	B2	20030130		
EP 1112262	A1	20010704	EP 1999-941351	19990909
EP 1112262	B1	20040804		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002524456	T	20020806	JP 2000-568841	19990909
AT 272628	T	20040815	AT 1999-941351	19990909
ES 2226422	T3	20050316	ES 1999-941351	19990909
MX 2001PA02539	A	20021017	MX 2001-PA2539	20010309
US 6458829	B1	20021001	US 2001-786949	20010511
US 2003186943	A1	20031002	US 2002-263336	20021001
US 6770658	B2	20040803		
PRIORITY APPLN. INFO.:			US 1998-99637P	P 19980909
			US 1999-121507P	P 19990223
			US 1999-149517P	P 19990817
			US 1999-393445	B1 19990908
			WO 1999-CA819	W 19990909
			US 2000-527699	B1 20000316
			US 2001-786949	A2 20010511
			US 2002-81993	A2 20020222
OTHER SOURCE(S):		MARPAT 132:222442		
GI				



AB The title compds. (I) [wherein R1 = W or R7(W)n; R2 = independently H, W, or R7(W)n; R7 = (halo)carbyl; n = 0-5; W = CONH2, CN, X, NO2, COX, N(R8)2, CO2R8, COR8, OCOR8, OR8, B(R8)2, B(OR8)2, P(R8)2, P(OR8)2, P(O)(OR8)2, SR8, SOR8, SO2R8, SON(R8)2, or SO2N(R8)2; X = halo; R8 = independently H or (halo)carbyl] and their lactams were prepared. Examples include syntheses for approx. 90 compds. and data from over 20 bioassays. For instance, II was prepared in a 12-step sequence involving: (1-9) formation of the tert-Bu (S)-5-hydroxy-4-[4-methoxy-3-(pentyloxy)phenyl]pentanoate intermediate starting from 3-hydroxy-4-methoxybenzyl alc., (10) ring closure to give the γ -phenyl- δ -lactone (94%), (11) α -addition of 4-(benzyloxy)-3-methoxybenzyl bromide (70%), and (12) debenzoylation of the alc. (83%). II inhibited neutrophil degranulation (IC50 < 1 μ M), displayed antioxidant activity against the radical cation ABTS+ (75-100% activity), inhibited resniferitoxin-induced mouse ear edema (98% by topical administration), and proved effective in reducing the effects of inflammatory bowel disease in rats and in treating existing rheumatoid arthritis in mice. Due to their antiinflammatory and antiproliferative activities, I are useful for the treatment of diseases such as rheumatoid

10/529290

arthritis, psoriasis, autoimmune disease, inflammatory bowel disease, asthma, graft vs. host disease, and cancer.

IC ICM C07D309-30

ICS C07F005-02; C07D405-10; C07F009-40; C07D211-76; A61K031-35

CC 27-13 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 1

IT 261357-66-8P 261357-73-7P 261357-79-3P 261357-86-2P 261357-94-2P
261357-98-6P 261358-05-8P 261358-07-0P 261358-09-2P 261358-12-7P
261358-14-9P 261358-15-0P 261358-16-1P 261358-21-8P
261358-23-0P 261358-28-5P 261358-35-4P 261358-40-1P 261358-42-3P
261358-44-5P 261358-46-7P 261358-48-9P 261358-50-3P 261358-51-4P
261358-53-6P 261358-54-7P 261358-55-8P 261358-68-3P 261358-69-4P
261358-70-7P 261358-71-8P 261358-72-9P 261358-73-0P 261358-74-1P
261358-75-2P 261358-76-3P 261358-77-4P 261358-78-5P 261358-80-9P
261358-81-0P 261358-83-2P 261358-90-1P 261358-91-2P 261358-92-3P
261358-93-4P 261358-94-5P 261358-95-6P 261358-96-7P 261358-97-8P
261358-98-9P 261358-99-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(target compound; preparation of substituted γ -phenyl- δ -lactones and lactams as antiinflammatory agents)

IT 261358-15-0P

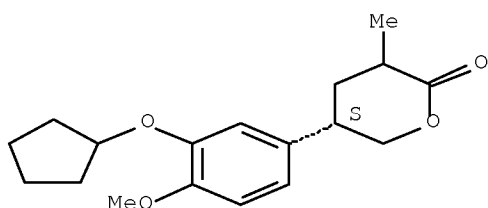
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(target compound; preparation of substituted γ -phenyl- δ -lactones and lactams as antiinflammatory agents)

RN 261358-15-0 ZCAPLUS

CN 2H-Pyran-2-one, 5-[3-(cyclopentyloxy)-4-methoxyphenyl]tetrahydro-3-methyl-, (5S)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L55 ANSWER 4 OF 26 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:503345 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 129:230608

TITLE: New Strategies in Carbonylation Chemistry: The Synthesis of δ -Lactones from Saturated Alcohols and CO

AUTHOR(S): Tsunoi, Shinji; Ryu, Ilhyong; Okuda, Tohru; Tanaka, Minoru; Komatsu, Mitsuo; Sonoda, Noboru

CORPORATE SOURCE: Department of Applied Chemistry Faculty of Engineering and Research Center for Environmental Preservation, Osaka University, Osaka, 565-0871, Japan

10/529290

SOURCE: Journal of the American Chemical Society (1998),
120(34), 8692-8701
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 129:230608

AB This paper describes the δ -carbonylation of saturated alcs. which uses a 1,5-hydrogen-transfer reaction of alkoxyl radicals and subsequent carbonylation at the δ -carbon atoms as the key. The carbonylation reactions of five classes of saturated alcs., namely, primary alcs. having primary δ -carbons, primary alcs. having secondary δ -carbons, primary alcs. having tertiary δ -carbons, secondary alcs. having primary δ -carbons, secondary alcs. having secondary δ -carbons, were carried out, in which lead tetraacetate (LTA) was used as a one-electron oxidant to generate the alkoxyl radicals. Carbonylation of these saturated alcs., except for primary alcs. having tertiary δ -carbons, took place to afford δ -lactones in moderate to good yields. The mechanism of the remote carbonylation likely involves (1) alkoxyl radical generation via LTA oxidation of a saturated alc., (2) conversion of this alkoxyl radical to a δ -hydroxyalkyl radical by a 1,5-hydrogen-transfer reaction, (3) CO trapping of the δ -hydroxyalkyl radical yielding an acyl radical, and (4) oxidation and cyclization of the acyl radical to give a δ -lactone. A metal salt-free system was also tested for a substrate derived from a tertiary alc. having a secondary δ -carbon; the photolysis of an alkyl 4-nitrobenzenesulfonate under CO pressures gave a δ -lactone in moderate yield.

CC 27-13 (Heterocyclic Compounds (One Hetero Atom))

IT 698-76-0P 1004-29-1P 1121-84-2P 14983-21-2P 16429-09-7P
22791-77-1P 24405-13-8P 24405-14-9P 65451-94-7P 65451-95-8P
82390-70-3P 99978-13-9P 142636-30-4P 142636-31-5P 156458-68-3P
156458-70-7P 156458-71-8P 156458-72-9P 156458-73-0P 156458-74-1P
156458-75-2P 156458-76-3P 156458-77-4P 212894-12-7P 212894-13-8P
212894-14-9P 212894-15-0P 212894-16-1P 212894-18-3P
212894-20-7P 212894-22-9P 212894-33-2P 212894-35-4P 212894-40-1P
212894-43-4P 212894-49-0P 212894-52-5P 212894-53-6P
212894-54-7P 212894-55-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of δ -lactones by carbonylation of saturated alcs.)

IT 212894-14-9P 212894-53-6P

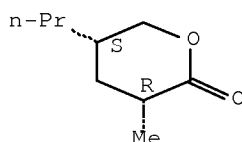
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of δ -lactones by carbonylation of saturated alcs.)

RN 212894-14-9 ZCAPLUS

CN 2H-Pyran-2-one, tetrahydro-3-methyl-5-propyl-, (3R,5S)-rel- (CA INDEX NAME)

Relative stereochemistry.



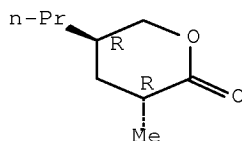
RN 212894-53-6 ZCAPLUS

CN 2H-Pyran-2-one, tetrahydro-3-methyl-5-propyl-, (3R,5R)-rel- (CA INDEX NAME)

10/529290

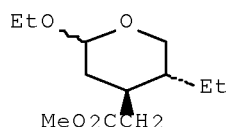
NAME)

Relative stereochemistry.

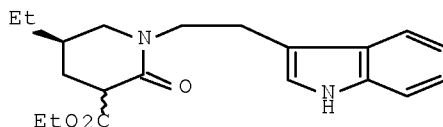


REFERENCE COUNT: 165 THERE ARE 165 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L55 ANSWER 5 OF 26 ZCAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1996:26683 ZCAPLUS Full-text
 DOCUMENT NUMBER: 124:146549
 TITLE: Synthesis of six-membered compounds by environmentally friendly cyclization using indirect electrolysis
 AUTHOR(S): Ihara, Masataka; Katsumata, Akira; Setsu, Fumihito; Tokunaga, Yuji; Fukumoto, Keiichiro
 CORPORATE SOURCE: Pharmaceutical Institute, Tohoku University, Aobayama, 980-77, Japan
 SOURCE: Journal of Organic Chemistry (1996), 61(2), 677-84
 CODEN: JOCEAH; ISSN: 0022-3263
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 124:146549
 GI



I



II

AB [Ni(cyclam)](ClO4)2-catalyzed indirect electroredn. of olefinic bromides produced six-membered compds. in low to high yields. The synthetic intermediate I of Ipecac and Corynanthe alkaloids was obtained in 88% yield in a highly stereoselective manner. Lactam II, the synthetic precursor of tacamonine, was prepared in 49% yield as a mixture of two diastereoisomers. The electrolysis of the bromoacetates gave the debrominated compds. in good yields.

CC 31-5 (Alkaloids)

Section cross-reference(s): 27, 72

IT 94844-37-8P 122937-63-7P 122937-67-1P 155529-27-4P 155529-33-2P
 157405-11-3P 163457-30-5P 163457-31-6P 163457-40-7P 163513-91-5P
 163513-92-6P 173423-60-4P 173423-61-5P 173423-62-6P 173423-64-8P
 173423-65-9P 173423-66-0P 173423-67-1P 173423-70-6P 173423-71-7P
 173423-72-8P 173423-78-4P 173423-80-8P 173423-81-9P

10/529290

173423-82-0P 173423-83-1P 173423-84-2P 173423-85-3P 173423-86-4P
 173423-87-5P 173423-88-6P 173423-89-7P 173423-90-0P 173423-91-1P
 173423-93-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (synthesis of six-membered compds. by electrochem. cyclization)

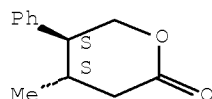
IT 173423-80-8P 173423-81-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (synthesis of six-membered compds. by electrochem. cyclization)

RN 173423-80-8 ZCAPLUS

CN 2H-Pyran-2-one, tetrahydro-4-methyl-5-phenyl-, trans- (9CI) (CA INDEX NAME)

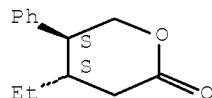
Relative stereochemistry.



RN 173423-81-9 ZCAPLUS

CN 2H-Pyran-2-one, 4-ethyltetrahydro-5-phenyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L55 ANSWER 6 OF 26 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1974:520459 ZCAPLUS [Full-text](#)

DOCUMENT NUMBER: 81:120459

ORIGINAL REFERENCE NO.: 81:19039a,19042a

TITLE: Epimeric mixtures of the lactone 3,6-dihydro-4,5-dimethyl-5-phenyl- α -pyrone

INVENTOR(S): Van Venrooy, John J.

PATENT ASSIGNEE(S): Sun Research and Development Co.

SOURCE: U.S., 3 pp. Continuation-in-part of U.S. 3,761,530 (CA 79;146293a).

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

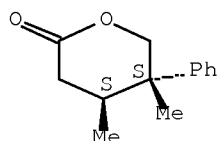
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
US 3825572	A	19740723	US 1972-318359	19721226
US 3761530	A	19730925	US 1972-258282	19720531
PRIORITY APPLN. INFO.:			US 1972-258282	A 19720531

GI For diagram(s), see printed CA Issue.

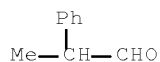
10/529290

AB Ph-CHMeCHO was treated with MeCHO and NaOH to give Ph- CHMeCH:C(CHO)CH:CMcPh
and a mixture of the 2 epimers of the pyranone I.
IC C07D
INCL 260343500
CC 27-13 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 25
IT 53655-81-5P 53655-82-6P 53855-97-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 93-53-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with acetaldehyde)
IT 53655-81-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 53655-81-5 ZCAPLUS
CN 2H-Pyran-2-one, tetrahydro-4,5-dimethyl-5-phenyl-, trans- (9CI) (CA INDEX
NAME)

Relative stereochemistry.



IT 93-53-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with acetaldehyde)
RN 93-53-8 ZCAPLUS
CN Benzeneacetaldehyde, α -methyl- (CA INDEX NAME)

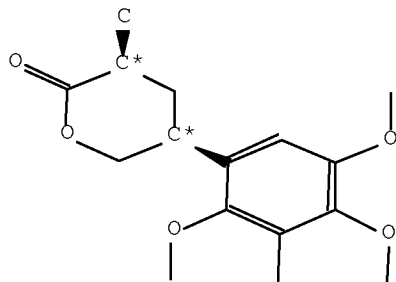


L55 ANSWER 7 OF 26 BEILSTEIN COPYRIGHT 2008 BEILSTEIN MDL on STN

Beilstein Records (BRN):	9208998
Chemical Name (CN):	(3S,5S)-3-methyl-5-(2,4,5-trimethoxy-3-methylphenyl)tetrahydropyran-2-one
Autonom Name (AUN):	3-methyl-5-(2,4,5-trimethoxy-3-methylphenyl)-tetrahydro-pyran-2-one
Molec. Formula (MF):	C16 H22 O5
Molecular Weight (MW):	294.35
Lawson Number (LN):	19213, 289
File Segment (FS):	Stereo compound

10/529290

Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 7776828
 Tautomer ID (TAUTID): 8646574
 Entry Date (DED): 2003/01/18
 Update Date (DUPD): 2003/01/18



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1
MS	Mass Spectrum	1
NMR	Nuclear Magnetic Resonance	3
ORP	Optical Rotatory Power	1

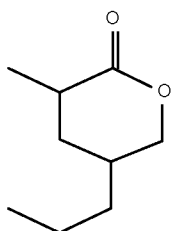
This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

All References:
 ALLREF

1. Heckrodt, Thilo J.; Mulzer, Johann, Synthesis, CODEN: SYNTBF(13), <2002>, 1857 - 1866; BABS-6363092

Beilstein Records (BRN): 8049582
 Chemical Name (CN): 3-methyl-5-propyl-tetrahydro-pyran-2-one
 Autonom Name (AUN): 3-methyl-5-propyl-tetrahydro-pyran-2-one
 Molec. Formula (MF): C9 H16 O2
 Molecular Weight (MW): 156.22
 Lawson Number (LN): 17736
 Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 6782509
 Tautomer ID (TAUTID): 7529184
 Beilstein Citation (BSO): 6-17
 Entry Date (DED): 1999/05/06
 Update Date (DUPD): 1999/05/07



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
IR	Infrared Spectrum	1
NMR	Nuclear Magnetic Resonance	3

This substance also occurs in Reaction Documents:

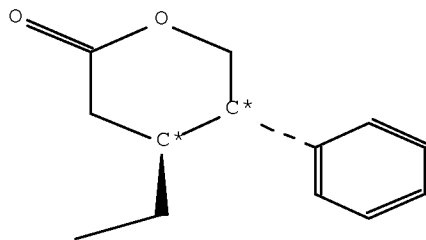
Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

All References:
 ALLREF

1. Tsunoi, Shinji; Ryu, Ilhyong; Okuda, Tohru; Tanaka, Minoru; Komatsu, Mitsuo; Sonoda, Noboru, J.Amer.Chem.Soc., CODEN: JACSAT, 120(34), <1998>, 8692-8701; BABS-6127724

L55 ANSWER 9 OF 26 BEILSTEIN COPYRIGHT 2008 BEILSTEIN MDL on STN

Beilstein Records (BRN): 7425194
 Chemical Name (CN): (+/-)-(3R*,4R*)-3-ethyl-4-phenyl-5-pentanolide
 Autonom Name (AUN): 4-ethyl-5-phenyl-tetrahydro-pyran-2-one
 Molec. Formula (MF): C13 H16 O2
 Molecular Weight (MW): 204.27
 Lawson Number (LN): 17953
 File Segment (FS): racemate, Stereo compound
 Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 6326546
 Tautomer ID (TAUTID): 7019664
 Beilstein Citation (BSO): 6-17
 Entry Date (DED): 1996/08/09
 Update Date (DUPD): 1997/04/28



Fragment Notes:

Additionally represents mirror image
 Stereo Descriptor: +/-

Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
FS	File Segment	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
IR	Infrared Spectrum	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

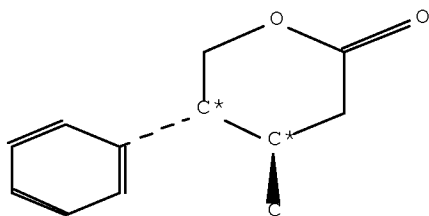
All References:

ALLREF

1. Ihara, Masataka; Katsumata, Akira; Setsu, Fumihito; Tokunaga, Yuji; Fukumoto, Keiichiro, J.Org.Chem., CODEN: JOCEAH, 61(2), <1996>, 677-684; BABS-6004130

L55 ANSWER 10 OF 26 BEILSTEIN COPYRIGHT 2008 BEILSTEIN MDL on STN

Beilstein Records (BRN): 7423599
 Chemical Name (CN): (+/-)-(3R*,4R*)-3-methyl-4-phenyl-5-pentanolide
 Autonom Name (AUN): 4-methyl-5-phenyl-tetrahydro-pyran-2-one
 Molec. Formula (MF): C12 H14 O2
 Molecular Weight (MW): 190.24
 Lawson Number (LN): 17944
 File Segment (FS): racemate, Stereo compound
 Compound Type (CTYPE): heterocyclic
 Constitution ID (CONSID): 6325158
 Tautomer ID (TAUTID): 7015418
 Beilstein Citation (BSO): 6-17
 Entry Date (DED): 1996/08/09
 Update Date (DUPD): 1997/04/28



Fragment Notes:

Additionally represents mirror image

Stereo Descriptor: +/-

Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1

10/529290

FW	Formular Weight	1
LN	Lawson Number	1
FS	File Segment	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
IR	Infrared Spectrum	1
MP	Melting Point	1
NMR	Nuclear Magnetic Resonance	2

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

All References:

ALLREF

1. Ihara, Masataka; Katsumata, Akira; Setsu, Fumihito; Tokunaga, Yuji; Fukumoto, Keiichiro, J.Org.Chem., CODEN: JOCEAH, 61(2), <1996>, 677-684; BABS-6004130

L55 ANSWER 11 OF 26 MARPAT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 146:280341 MARPAT Full-text

TITLE: Hair-styling conditioners containing dicarboxylic acids, organic solvents, and royal jelly, and method of hair modification using them

INVENTOR(S): Ueno, Masako; Kamiyama, Kenichi

PATENT ASSIGNEE(S): Kao Corp., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 15pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

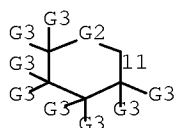
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2007055918	A	20070308	JP 2005-241664	20050823
PRIORITY APPLN. INFO.:			JP 2005-241664	20050823

AB The hair-styling conditioners contain (A) (OH-containing) C₈ organic dicarboxylic acids or their salts, (B) organic solvents (ClogP -2 to +3) selected from aromatic alcs., N-alkylpyrrolidones, alkylene carbonates, polypropylene glycol, lactones, and cyclic ketones, and (C) royal jelly or its exts. and show pH 2-5 at 25° when diluted 20-fold (by weight) with H₂O. The hair conditioners may also contain silicones, oily conditioners, and/or cationic surfactants. A composition (pH 3.7) containing malic acid 5.0, 2-benzyloxyethanol 2.5, glycerin 1.0, EtOH 10.0, royal jelly extract 2.0, NaOH (pH-adjusting agent), and H₂O to 100 weight% was applied on human hair and dried, showing hair-styling, -conditioning, and hair elasticity-improving effects. The effects lasted even after shampooing.

MSTR 2

G1=O

G1 = 11



G2 = O

G3 = alkyl (opt. substd. by G4) / Me

G4 = CO₂H

Patent location: disclosure

Note: substitution is restricted

L55 ANSWER 12 OF 26 MARPAT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 147:246792 MARPAT [Full-text](#)

TITLE: Stripping compositions and method for removing photoresists

INVENTOR(S): Yoon, Seok Il; Kim, Seong Bae; Chung, Jong Hyeon; Park, Hui Jin; Kim, Byeong Uk

PATENT ASSIGNEE(S): Dongjin Semichem Co., Ltd., S. Korea

SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 18pp.
CODEN: CNXXEV

DOCUMENT TYPE: Patent

LANGUAGE: Chinese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

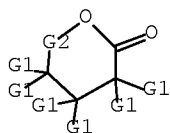
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 101000467	A	20070718	CN 2007-10000702	20070110
KR 2007074745	A	20070718	KR 2006-2682	20060110
JP 2007188081	A	20070726	JP 2007-2181	20070110
PRIORITY APPLN. INFO.:			KR 2006-2682	20060110

AB The compns. for use in lithog. process comprise (un)substituted lactone compds., organic acid or amine compds., and oxidants. The lactone compds. are selected from ≥ 1 of γ -butyrolactone, γ -methylene γ -butyrolactone, α -methyl- γ -butyrolactone, α -methylene γ -butyrolactone, 2-acetyl butyrolactone, γ -hexalactone, δ -hexalactone, γ -nonalactone, δ -octalactone, γ -valerolactone, and δ -valerolactone. The organic acid compds. are selected from ≥ 1 of benzoic acid, toluic acid, hydroxybenzoic acid, aminobenzoic acid, citric acid, succinic acid, hydroxy succinic acid, maleic acid, salicylic acid, oxalic acid, phthalic acid, itaconic acid, succinic anhydride, and itaconic anhydride. The organic amines are selected from ≥ 1 of dimethylethanolamine, diethylmethanolamine, diethylethanolamine, Me diethanolamine, Et dimethanolamine, Et diethanolamine, trimethanolamine, triethanolamine, etc.

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The oxidants are selected from ≥ 1 of H₂O₂, tert-Bu hydrogen peroxide, benzoyl hydrogen peroxide, etc. The compns. have excellent stripping effect and cause no corrosion to patterned metal films.

MSTR 2



G1 = Me / Pr-n
G2 = 13



Patent location: claim 1

L55 ANSWER 13 OF 26 MARPAT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 146:86862 MARPAT [Full-text](#)

TITLE: Hair conditioners containing cationic surfactants or tertiary amines, fatty alcohols, and toluenesulfonates

INVENTOR(S): Tokunaga, Shinichi

PATENT ASSIGNEE(S): Kao Corp., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 15pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2006347997	A	20061228	JP 2005-179589	20050620
US 2007071709	A1	20070329	US 2006-454934	20060619
CN 1891189	A	20070110	CN 2006-10093089	20060620
EP 1754516	A2	20070221	EP 2006-12670	20060620
EP 1754516	A3	20070815		

R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU

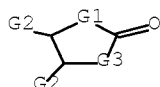
PRIORITY APPLN. INFO.: JP 2005-179589 20050620

AB The hair conditioners [pH (at 25°) of 20-fold (by weight) aqueous dilution 1-5.5] contain (A) cationic surfactants and/or tertiary amines R₁(AR₄)aNR₂R₃ [≥ 1 of R₁-R₃ is (are) C₈-23 aliphatic hydrocarbonyl; the rest of R₁-R₃ is (are) H, C₁-6 alkyl, hydroxyalkyl, benzyl; R₄ = C₁-6 alkylene; A = CONH, NHCO; a = 0, 1] or their salts, (B) C₈-30 fatty alcs., and (C) toluenesulfonic acid or its salts. The hair conditioners may also contain specific organic solvents. An

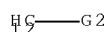
10/529290

aqueous hair conditioner composition (pH 3.5) containing stearyltrimethylammonium chloride 1.5, stearyl alc. 3, behenyl alc. 3, p-toluenesulfonic acid 0.1 weight%, etc., was effective for recovery of hair damaged by bleaching.

MSTR 3



G1 = O
G2 = alkyl (substd. by CO₂H) / Me
G3 = (1-3) 12



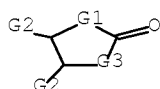
Patent location: claim 2
Note: substitution is restricted

L55 ANSWER 14 OF 26 MARPAT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 145:425245 MARPAT Full-text
TITLE: Conditioning shampoos containing amino-modified
silicones and hydrophobic sulfonic acids
INVENTOR(S): Tokunaga, Shinichi
PATENT ASSIGNEE(S): Kao Corp., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 18pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

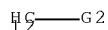
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2006282615	A	20061019	JP 2005-106452	20050401
PRIORITY APPLN. INFO.:			JP 2005-106452	20050401

AB This invention relates to shampoos for damaged hair which provide excellent foamability, rinsability, and textures in high humidity. The shampoos (pH 2-6) comprise (1) amino-modified silicones, (2) hydrophobic sulfonic acids or salts thereof, (3) hydroxycarboxylic acids, dicarboxylic acids, and/or aromatic carboxylic acids, and (4) organic solvents. For example, a shampoo (pH 3.7) contained amino-modified silicone (Conditioning agent 8500) 0.3, p-toluenesulfonic acid 0.5, malic acid 0.5, lactic acid 0.2, ethanol 0.5, benzyl alc. 0.5, polypropylene glycol 0.3, PEG lauryl ether sulfate Na salt 12, amidopropylbetaine 2, PEG lauryl ether 1, cationic hydroxyethyl cellulose 0.5, Merquat 550 0.2, Silicone CF2450 2, KT1989 0.3, myristyl alc. 0.5, NaOH 0.2, and distilled water balance to 100 %.

MSTR 2



G1 = O
 G2 = alkyl (substd. by CO₂H) / Me
 G3 = (1-3) 12



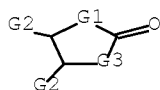
Patent location: claim 1
 Note: substitution is restricted

L55 ANSWER 15 OF 26 MARPAT COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 145:425244 MARPAT [Full-text](#)
 TITLE: Shampoos containing hydrophobic sulfonic acids
 INVENTOR(S): Tokunaga, Shinichi
 PATENT ASSIGNEE(S): Kao Corp., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 16pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2006282613	A	20061019	JP 2005-106450	20050401
PRIORITY APPLN. INFO.:			JP 2005-106450	20050401

AB This invention relates to shampoos for damaged hair which provide excellent dry hair combability. The shampoos (pH 2-6) comprise (1) monoalkyl glyceryl ethers or monoalkenyl glyceryl ethers, (2) hydrophobic sulfonic acids or salts thereof, (3) hydroxycarboxylic acids, dicarboxylic acids, and/or aromatic carboxylic acids, and (4) organic solvents. For example, a shampoo (pH 3.7) contained isodecyl glyceryl ether 1, p-toluenesulfonic acid 0.5, malic acid 0.5, lactic acid 0.2, ethanol 0.5, benzyl alc. 0.5, polypropylene glycol 0.3, PEG lauryl ether sulfate Na salt 12, amidopropylbetaine 2, PEG lauryl ether 1, cationic hydroxyethyl cellulose 0.5, Merquat 550 0.2, Silicone CF2450 2, KT1989 0.3, myristyl alc. 0.5, NaOH 0.2, and distilled water balance to 100 %.

MSTR 2



10/529290

G1 = 0
G2 = alkyl (substd. by CO2H) / Me
G3 = (1-3) 12

H5—G2

Patent location: claim 1
Note: substitution is restricted

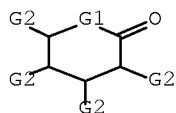
L55 ANSWER 16 OF 26 MARPAT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 145:382947 MARPAT Full-text
TITLE: Hair cleansing composition comprising a sulfate
surfactant, a sulfonate, and a carboxylate
INVENTOR(S): Tokunaga, Shinichi
PATENT ASSIGNEE(S): Kao Corporation, Japan
SOURCE: Eur. Pat. Appl., 21 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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EP 1707239	A2	20061004	EP 2006-6960	20060331
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, BA, HR, IS, YU				
JP 2006282614	A	20061019	JP 2005-106451	20050401
CN 1853600	A	20061101	CN 2006-10066912	20060330
US 2006223728	A1	20061005	US 2006-393921	20060331
PRIORITY APPLN. INFO.:			JP 2005-106451	20050401

AB The invention relates to a hair cleansing composition comprising (A) a sulfate surfactant, (B) a C6-18 hydrophobic sulfonic acid or salt thereof, (C) a hydroxycarboxylic acid, dicarboxylic acid or aromatic carboxylic acid, and (D) an organic solvent; and having a pH of 2 to 6. A sulfate surfactant, represented by the formula R1-O-(C2H4O)n-SO3M (R1 = C10-18 alkyl or alkenyl; n = 0 or a pos. integer; M = ammonium, Na) is composed of 30 to 45 weight% of a sulfate exhibiting n = 0, 18 to 27 weight% of a sulfate exhibiting n = 1, 10 to 20 weight% of a sulfate exhibiting n = 2, and the balance of sulfates exhibiting n = 3 or greater, and containing the sulfates exhibiting n = 0 to 2 in a total amount of 70 weight% or greater based on the total sulfates,. The hair cleansing composition according to the present invention is excellent in the hair feel during shampooing and effects for straightening the flyaway or waved hair tip, which has resulted from the accumulation of damages caused, for example, by hair coloring. Thus, a hair cleansing composition was prepared containing ammonium lauryl ether sulfate with an average of 1.0 mol of EO (preparation given) 48, p-toluenesulfonic acid 0.5, malic acid 0.5, ethanol 0.5, benzyl alc. 0.5, polypropylene glycol 0.3, amidopropylbetaine 2, cocoylmonoethanolamide 1, polyoxyethylene lauryl ether 0.8, cationic hydroxyethyl cellulose 0.5, Merquat 550 0.2, Silicone CF2450 2, amino-modified silicone KT1989 0.3, myristyl alc. 0.5, ethylene glycol distearate 2, KOH as needed for pH 3.7, and water to 100 weight%, resp.

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MSTR 4



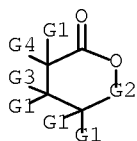
G1 = O
 G2 = alkyl (substd. by CO₂H) / Me
 Patent location: claim 1
 Note: substitution is restricted

L55 ANSWER 17 OF 26 MARPAT COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 143:45571 MARPAT Full-text
 TITLE: Compositions containing lactone compatibilizers
 INVENTOR(S): Fagan, Paul Joseph; Minor, Barbara Haviland; Shuey, Steven W.; Mahler, Walter
 PATENT ASSIGNEE(S): USA
 SOURCE: U.S. Pat. Appl. Publ., 24 pp.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005127321	A1	20050616	US 2004-965322	20041014
PRIORITY APPLN. INFO.:			US 2003-511881P	20031015

AB The present invention relates to compns. that are useful for compatibilizing a conventional compression refrigeration lubricant and a hydrofluorocarbon and/or hydrochlorofluorocarbon refrigerant in a compression refrigeration or air conditioning system. Addnl., these compns. promote efficient return of lubricant from the non-compressor zones to the compressor zones of refrigeration and air conditioning systems.

MSTR 1



G1 = Pr-n
 G2 = 16

10/529290



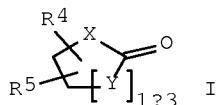
G3 = Me

Patent location: claim 1

L55 ANSWER 18 OF 26 MARPAT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 140:222914 MARPAT Full-text
TITLE: Storage-stable acidic conditioning shampoo
compositions with good foamability for imparting
gloss, smoothness, and wet feel to hair
INVENTOR(S): Terasaki, Hiroyuki
PATENT ASSIGNEE(S): Kao Corp., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 15 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004075545	A	20040311	JP 2002-233706	20020809
JP 3843051	B2	20061108		
PRIORITY APPLN. INFO.:			JP 2002-233706	20020809

GI



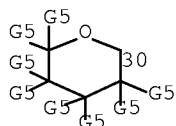
AB Title compns. contain (A) dicarboxylic acids, hydroxycarboxylic acids, or their salts, (B) organic solvents chosen from R1(OCH2CH2)p[OCH2CH((CH2)rY)]qZ [R1 = H, lower alkyl, 4-R2C6H4R3; R2 = H, Me, MeO; R3 = bond, C1-3 (un)saturated divalent hydrocarbylene; Y, Z = H, OH; p, q, r = 0-5; when p = q = 0, then Z ≠ H and R1 = alkyl], N-C1-18 alkylpyrrolidone, C1-4 alkylene carbonates, polypropylene glycol with mo. weight 200-5000, and lactones or cyclic ketones I (X = CH2, O; R4, R5 = substituent; R4 ≠ R5; a, b = 0, 1; s = 1-3), (C) sulfate-type anionic surfactants, and (D) vitamins, amino acids, amino acid analogs, protein hydrolyzates, or their derivs., and show pH 1-4 at 25° when 20-fold diluted in water. Thus, a shampoo (pH 3.5 when 20-fold diluted in water) containing malic acid, benzyloxyethanol, polyoxyethylene lauryl ether sulfate Na salt, Na lauryl sulfate, panthenol, and pantothenyl Et ether showed good hair treatment effect and no change when stored at 50° for 1 mo.

MSTR 1

10/529290

G1=O

G1 = 30



G5 = alkyl (substd. by G8) / Me

G8 = CO₂H

Patent location: claim 1

Note: substitution is restricted

L55 ANSWER 19 OF 26 MARPAT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 140:222871 MARPAT Full-text

TITLE: Storage-stable acidic conditioning shampoo compositions with good foamability for imparting gloss and softness to hair

INVENTOR(S): Terasaki, Hiroyuki

PATENT ASSIGNEE(S): Kao Corp., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 2004075544	A	20040311	JP 2002-233705	20020809
JP 3964759	B2	20070822		

PRIORITY APPLN. INFO.: JP 2002-233705 20020809

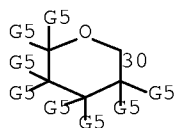
AB Title compns. contain sulfate-type anionic surfactants, cationic polymers, and inorg. acids or their salts, and show pH 1-4 at 25° when 20-fold diluted in water. Thus, a shampoo (pH 3.5 when 20-fold diluted in water) containing polyoxyethylene lauryl ether sulfate Na salt, Na lauryl sulfate, cationized cellulose, cationized guar gum, and HCl showed good hair treatment effect and no change when stored at 50° for 1 mo.

MSTR 1

G1=O

10/529290

G1 = 30



G5 = alkyl (substd. by G8) / Me

G8 = CO₂H

Patent location: claim 1

Note: substitution is restricted

L55 ANSWER 20 OF 26 MARPAT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 136:279325 MARPAT Full-text

TITLE: Preparation and use of amido-lactone integrin antagonists

INVENTOR(S): Ruminiski, Peter; Penning, Thomas D.; Jiang, Lan; Balekudru, Devadas; Rogers, Thomas; Yuan, Chester; Vancamp, Jennifer

PATENT ASSIGNEE(S): Pharmacia Corporation, USA

SOURCE: PCT Int. Appl., 88 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

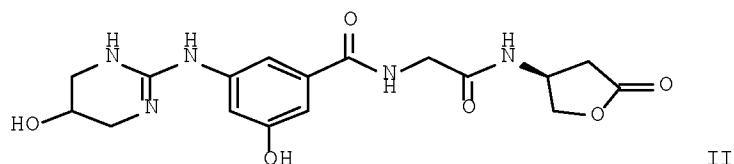
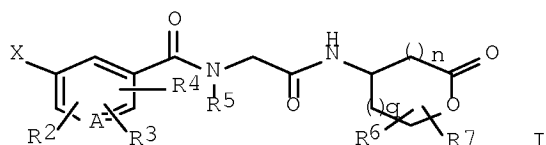
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

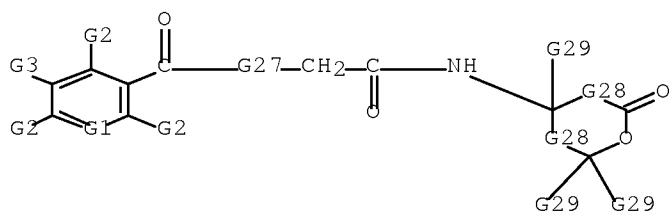
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002026227	A1	20020404	WO 2001-US30194	20010927
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2002045645	A1	20020418	US 2001-963926	20010926
US 6720327	B2	20040413		
CA 2423434	A1	20020404	CA 2001-2423434	20010927
AU 2001094776	A5	20020408	AU 2001-94776	20010927
EP 1320363	A1	20030625	EP 2001-975450	20010927
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004513088	T	20040430	JP 2002-530057	20010927
US 2004019206	A1	20040129	US 2003-381831	20030327
US 2004116472	A1	20040617	US 2003-717238	20031119
US 6906051	B2	20050614		
PRIORITY APPLN. INFO.:			US 2000-235617P	20000927
			US 2000-241633P	20001010
			US 2001-963926	20001010
			WO 2001-US30194	20010927

GI



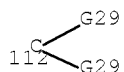
AB Title compds. I [X = NHC:YNR₈R₉, NHC:NR₁NR₈R₉, etc.; Y = NR₁, O, S; p, q = 0-3; A = N, C; R₁ = H, alkyl, aryl, hydroxy, alkoxy, cyano, nitro, amino, alkenyl, alkynyl, amido, etc. or R₁ taken together with R₈ forms a 4-12 membered heterocycle; R₈ (when not taken together with R₁), R₉ = H, alk(en/yn)yl, aralkyl, amino, alkylamino, hydroxy, alkoxy, arylamino, amido, alkylcarbonyl, arylcarbonyl, alkoxycarbonyl, aryloxy, aryloxycarbonyl, haloalkylcarbonyl, haloalkoxycarbonyl, alkylthiocarbonyl, arylthiocarbonyl, acyloxymethoxycarbonyl, etc. or NR₈ and R₉ taken together form a 4-12 membered heterocycle; R₂-4 = H, alkyl, hydroxy, alkoxy, aryloxy, halogen, haloalkyl, haloalkoxy, nitro, amino, alkylamino, acylamino, dialkylamino, cyano, alkylthio, etc.; R₅-7 = H, alk(en/yn)yl, aryl, carboxy derivs., haloalkyl, cycloalkyl, monocyclic heterocycles, monocyclic heterocycles optionally substituted with alkyl, halogen, haloalkyl, cyano, hydroxy, aryl, fused aryl, nitro, alkoxy, aryloxy, alkylsulfonyl, arylsulfonyl, sulfonamide, thio, alkylthio, carboxy derivs., amino, amido, etc.] were prepared. For instance, (4S)-4-aminodihydro-2(3H)furanone hydrochloride (preparation given) was reacted with Boc-Gly-OSu (DMF, NMM, 0°C, 18 h) and the product deprotected with 4N HCl. The intermediate amine was condensed with the corresponding carboxylic acid (prior art, DMF, CH₂Cl₂, DCC, NMM, 18 h) to give II isolated as the TFA salt. Example compds. had IC₅₀ = 0.1 nM - 100 nM for the αvβ3 integrin and IC₅₀ < 50 μM for the αvβ5 integrin. I are useful for the treatment of tumor metastasis, solid tumor growth, macular degeneration, etc.

MSTR 1



10/529290

G28 = (0-3) 112



G29 = alkyl <containing 1-10 C> (substd. by CO₂H) / Me

Patent location: claim 1

Note: and tautomers and polymorphs

Stereochemistry: and isomers, enantiomers and racemates

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L55 ANSWER 21 OF 26 MARPAT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 138:14020 MARPAT Full-text

TITLE: Preparation of a lactam aldehyde compound

INVENTOR(S): Izumi, Hiroshi; Futamura, Shigeru

PATENT ASSIGNEE(S): Director-General of National Institute of Advanced Industrial Science and Technology, Japan

SOURCE: Eur. Pat. Appl., 10 pp.

CODEN: EPXXDW

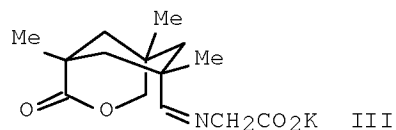
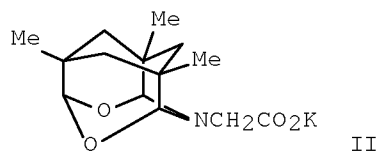
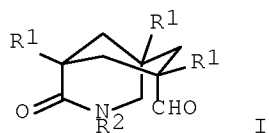
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

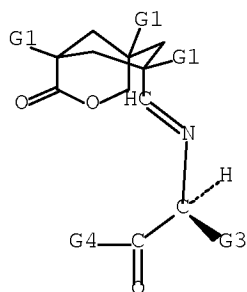
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1262479	A1	20021204	EP 2002-251706	20020311
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2002356476	A	20021213	JP 2001-159742	20010528
JP 3774763	B2	20060517		
US 2002198386	A1	20021226	US 2002-91459	20020307
US 6639075	B2	20031028		
PRIORITY APPLN. INFO.:			JP 2001-159742	20010528
GI				



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AB A lactam aldehyde I [R1 = alkyl; R2 = CHR3COR4; R3 = H, amino acid side chain; R4 = OH, peptide side chain, salt of OH] were prepared for use as mol. recognition agents in neurotransmission studies, intermediates for protein analogs, surfactants, protective groups, or hosts for host-guest complexes (no data). Thus, the dioxazawurtzitane II was rearranged to the lactone imine III by treatment with aqueous MeCN at room temperature for 3 days. III was then stirred in Me2SO at room temperature for 5 days to give I [R1 = Me, R2 = CH2CO2H].

MSTR 2



G1 = Me / Pr-n

Patent location: claim 5

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L55 ANSWER 22 OF 26 MARPAT COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 132:278654 MARPAT Full-text
 TITLE: Emulsifiers for fertilizer emulsion compositions
 INVENTOR(S): Bush, James H.
 PATENT ASSIGNEE(S): Lubrizol Corp., USA
 SOURCE: U.S., 17 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6054493	A	20000425	US 1998-222662	19981230
CA 2357040	A1	20000713	CA 1999-2357040	19991215
WO 2000040327	A1	20000713	WO 1999-US29686	19991215
W: AU, CA				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 1140346	A1	20011010	EP 1999-965261	19991215
EP 1140346	B1	20040317		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
AU 769406	B2	20040129	AU 2000-31214	19991215

10/529290

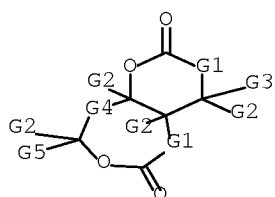
PRIORITY APPLN. INFO.:

US 1998-222662 19981230

WO 1999-US29686 19991215

AB Nonexplosive fertilizer emulsion compns. comprise an aqueous phase (e.g., containing NH_4NO_3 , $\text{Zn}(\text{NO}_3)_2$, urea), an organic phase, and an emulsifier composition comprising the reaction product of an amine having ≥ 1 NH group and an intermediate formed in the reaction of ≥ 1 olefinic compound (e.g., polyisobutene) containing ≥ 1 C=CCH group and ≥ 1 carboxylic reactant (e.g., glyoxylic acid) selected from compds. of formula $\text{R}_3\text{C}(\text{O})(\text{R}_4)_n\text{C}(\text{O})\text{OR}_5$ where R_3, R_5 are sep. H, hydrocarbyl; R_4 is a divalent hydrocarbyl group; n is 0 or 1; and ≥ 1 aldehyde (e.g, formaldehyde) or ketone.

MSTR 4



G1 = bond

G2 = Me

G4 = CH_2 (opt. substd. by G7)

G7 = Pr-n

Patent location: claim 23

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L55 ANSWER 23 OF 26 MARPAT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 132:207762 MARPAT Full-text

TITLE: Preparation of pyranones

INVENTOR(S): Abe, Nobuki

PATENT ASSIGNEE(S): Nippon Zeon Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.

CODEN: JKXXAF

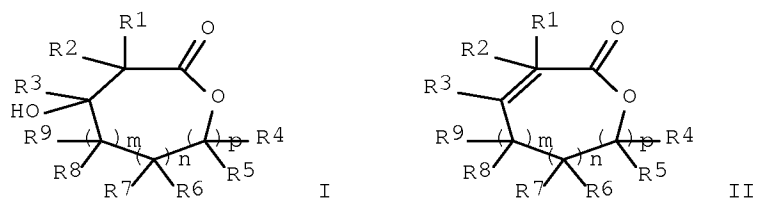
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

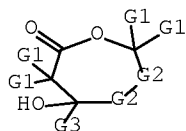
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 2000080090	A	20000321	JP 1998-247563	19980901
PRIORITY APPLN. INFO.:			JP 1998-183787	19980630
OTHER SOURCE(S):		CASREACT 132:207762		
GI				

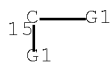


AB Title compds. I (R1-R2, R4-R9 = H, NO₂, cyano, C1-6 alkyl, alkenyl, aryl; R3 = H, C1-6 alkyl, alkenyl, aryl; m, n, p = 0-1; m = n = p ≠ 0) or II (R2, R4-R9, R3, m, n, p = same as I) are prepared by cyclization of XCR₁R₂CO₂(CR₄R₅)_r(CR₆R₇)_s(CR₈R₉)_tCOR₃ (X = halo; R1-R9, m, n, p = same as I) in the presence of transition metals. 3-Oxobutyl bromoacetate (preparation given) was cyclized in the presence of Zn and I in C₆H₆ under heating for 80 min to give 76% mevalonolactone.

MSTR 2



G1 = Pr-n
G2 = 15

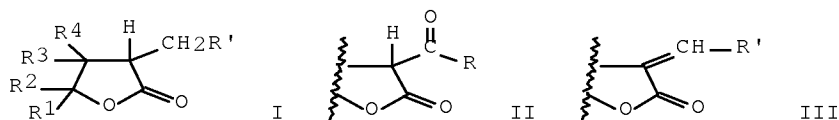


G3 = Me

Patent location: claim 1

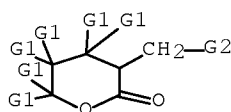
L55 ANSWER 24 OF 26 MARPAT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 117:212305 MARPAT Full-text
TITLE: Process for the preparation of α -alkyl lactones,
useful as aroma chemicals, from α -acyl lactones
INVENTOR(S): Rebrovic, Louis; Harris, Eugene G.
PATENT ASSIGNEE(S): Henkel K.-G.a.A., USA
SOURCE: PCT Int. Appl., 48 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9209590	A1	19920611	WO 1991-US8745	19911125
W: JP				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
DE 4027241	A1	19910307	DE 1990-4027241	19900829
GB 2235451	A	19910306	GB 1990-19012	19900831
FR 2651496	A1	19910308	FR 1990-10899	19900831
NL 9001922	A	19910402	NL 1990-1922	19900831
JP 03130276	A	19910604	JP 1990-232287	19900831
US 5231192	A	19930727	US 1990-619797	19901129
EP 559789	A1	19930915	EP 1992-901529	19911125
R: BE, DE, FR, GB, IT, NL				
JP 06503328	T	19940414	JP 1992-501551	19911125
PRIORITY APPLN. INFO.:			US 1990-619797	19901129
			US 1989-315109	19890224
			US 1989-402105	19890901
			WO 1991-US8745	19911125
OTHER SOURCE(S):			CASREACT 117:212305	
GI				



AB α -Alkyl- γ -butyrolactones I (R1-R4, R' = H, C1-20 hydrocarbyl), useful in fragrances, are prepared in 2 steps: (A) reaction of acyl lactones II (R = C1-8 alkyl) with aldehydes R'CHO and alkali metal hydroxides at 50-150° in an inert diluent while removing H₂O of reaction, and (B) selective hydrogenation of the formed alkylidene lactones III. Similar preparation of α -alkyl- δ -valerolactones is also claimed. For example, II (R = R1 = Me; R2-R4 = H) (prepared from Et acetoacetate and propylene oxide) was refluxed with heptaldehyde and NaOH under Dean-Stark conditions in PhMe to give 54.5% III [R' = (CH₂)₅Me; R1-R4 as given], which was hydrogenated over 5% Pd/C in EtOH to give 95% cis-I [R1 = Me; R2-R4 = H; R' = (CH₂)₅Me]. The latter, a preferred I, has a nutty, pecan odor.

MSTR 4



G1 = Ph (opt. substd. by alkyl <containing 1-8 C>)
 Patent location: claim 13

10/529290

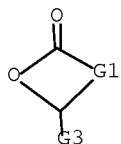
L55 ANSWER 25 OF 26 MARPAT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 118:59572 MARPAT Full-text
 TITLE: Preparation of lactones
 INVENTOR(S): Abe, Yutaka; Imoto, Hiroyuki; Sotodani, Koshiro
 PATENT ASSIGNEE(S): Kao Corp., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04261167	A	19920917	JP 1991-20708	19910214
JP 3021700	B2	20000315		
PRIORITY APPLN. INFO.:			JP 1991-20708	19910214
OTHER SOURCE(S): CASREACT 118:59572				

AB Lactones are prepared by dehydrocyclization of compds. having ≥ 2 OH, in which 2 OH are combines with (un)substituted 4-6 carbons, and one of the 2 OH is primary OH, in the presence of catalysts containing Cu, transition metals of 4th period and Pt-group elements. A mixture of 1,4-butanediol and a catalyst [prepared from Cu nitrate, $\text{Zn}(\text{NO}_3)_2$, and RuCl_3] was bubbled with H at 190° for 5 h to give 97% γ -butyrolactone.

MSTR 2



G1 = (2-4) 6



G2 = Me / $\text{CH}_2\text{CH}=\text{CH}_2$

Patent location: disclosure

L55 ANSWER 26 OF 26 MARPAT COPYRIGHT 2008 ACS on STN

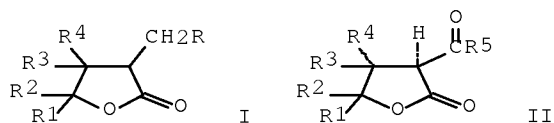
ACCESSION NUMBER: 114:101715 MARPAT Full-text
 TITLE: Preparation of α -alkyl lactones
 INVENTOR(S): Rebrovic, Louis; Harris, Eugene G.
 PATENT ASSIGNEE(S): Henkel Corp., USA
 SOURCE: Ger. Offen., 10 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent

10/529290

LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

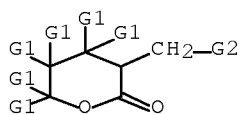
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4005515	A1	19900830	DE 1990-4005515	19900222
US 4980342	A	19901225	US 1989-402105	19890901
GB 2228481	A	19900829	GB 1990-4142	19900223
GB 2228481	B	19920415		
NL 9000443	A	19900917	NL 1990-443	19900223
JP 02273667	A	19901108	JP 1990-44309	19900223
BE 1003310	A5	19920225	BE 1990-200	19900223
FR 2643635	A1	19900831	FR 1990-2350	19900226
DE 4027241	A1	19910307	DE 1990-4027241	19900829
GB 2235451	A	19910306	GB 1990-19012	19900831
FR 2651496	A1	19910308	FR 1990-10899	19900831
NL 9001922	A	19910402	NL 1990-1922	19900831
JP 03130276	A	19910604	JP 1990-232287	19900831
PRIORITY APPLN. INFO.:			US 1989-315109	19890224
			US 1989-402105	19890901

GI



AB α -Alkyl butyrolactones I [R1, R2, R3, R4 = C1-8 alkyl, C3-6 cycloalkyl, (C1-8 alkyl)phenyl, (C1-8 alkyl)benzyl; R = H, C1-8 alkyl or alkenyl, C3-8 cycloalkyl or cycloalkenyl, (substituted) Ph or benzyl] and corresponding valerolactones were prepared by condensation of, e.g., α -acyl butyrolactones II (R5 = C1-8 alkyl) with RCHO in the presence of an alkali metal hydroxide, followed by catalytic hydrogenation. E.g., reaction of 3-acetyl-5-methyldihydro-2(3H)-furanone (III) with cyclohexanecarboxaldehyde in the presence of NaOH in refluxing PhCH₃, followed by hydrogenation using 5% Pt-C catalyst gave title compound I (R = cyclohexyl, R1 = Me, R2, R3, R4 = H) in 50% yield. III was prepared by alkylation and intramol. cyclization of Et acetoacetate with propylene oxide.

MSTR 4



G1 = Ph (opt. substd. by 1 or more alkyl <containing 1-8 C>)

10/529290

Patent location:

claim 12

10/529290

=> d his full

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FILE 'REGISTRY' ENTERED AT 16:29:23 ON 26 MAR 2008

L1 STRUCTURE UPLOADED
L2 STRUCTURE UPLOADED
L3 0 SEA SSS SAM L1 AND L2
L4 0 SEA SSS SAM L1

FILE 'ZCAPLUS' ENTERED AT 16:30:28 ON 26 MAR 2008

E US2005-529290 /APPS
L5 1 SEA ABB=ON PLU=ON US2005-529290 /AP
D SCA
SEL RN

FILE 'REGISTRY' ENTERED AT 16:31:30 ON 26 MAR 2008

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28219-60-5/BI OR 28219-61-6/BI OR 609-02-9/BI OR 623-36-9/BI
OR 65113-99-7/BI OR 677326-31-7/BI OR 677326-32-8/BI OR
677326-33-9/BI OR 677326-34-0/BI OR 677326-35-1/BI OR 677326-36
-2/BI OR 677326-37-3/BI OR 677326-38-4/BI OR 677326-39-5/BI OR
677326-40-8/BI OR 677326-41-9/BI OR 677326-42-0/BI OR 677326-43
-1/BI OR 677326-44-2/BI OR 677326-45-3/BI OR 677326-46-4/BI OR
677763-76-7/BI OR 677763-77-8/BI OR 67801-20-1/BI OR 72089-08-8
/BI OR 93-53-8/BI)
L7 14 SEA ABB=ON PLU=ON L6 AND OC5/ES
D SCA
D RN 1
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D L8
D STAT QUE L4
L9 16 SEA SSS FUL L1
SAVE TEMP L9 CHA290STR1L/A
L10 9 SEA ABB=ON PLU=ON L9 AND L7
L11 5 SEA ABB=ON PLU=ON L7 NOT L10
D SCA
L12 6097 SEA ABB=ON PLU=ON C10H18O2/MF
L13 1 SEA ABB=ON PLU=ON L11 AND L12

FILE 'ZCAPLUS' ENTERED AT 16:35:26 ON 26 MAR 2008

L14 7 SEA ABB=ON PLU=ON L9
L15 1 SEA ABB=ON PLU=ON L13 AND L14
L16 2 SEA ABB=ON PLU=ON L6 AND L14
D SCA

FILE 'BEILSTEIN' ENTERED AT 16:38:54 ON 26 MAR 2008

L17 0 SEA SSS SAM L1
L18 0 SEA SSS SAM L1 AND L2
L19 SCREEN 1338
L20 0 SEA SSS SAM L1 AND L19
L21 4 SEA SSS FUL L1 AND L19
L22 4 SEA ABB=ON PLU=ON L21/COM

FILE 'MARPAT' ENTERED AT 16:43:26 ON 26 MAR 2008

L23 5 SEA SSS SAM L1
L24 96 SEA SSS FUL L1

10/529290

L25 STRUCTURE UPLOADED

L26 0 SEA SUB=L24 SSS SAM L25

L27 17 SEA SUB=L24 SSS FUL L25

L28 112 SEA ABB=ON PLU=ON COSME?/BI

L29 112 SEA ABB=ON PLU=ON COSME?/BI,IT

L30 0 SEA ABB=ON PLU=ON L24 AND L28

FILE 'ZCAPLUS' ENTERED AT 16:52:32 ON 26 MAR 2008

L31 89969 SEA ABB=ON PLU=ON COSME?/BI

L32 36798 SEA ABB=ON PLU=ON ?PERFUM?/BI

L33 1 SEA ABB=ON PLU=ON L9 (L) COS/RL

L34 1 SEA ABB=ON PLU=ON L14 AND (L31 OR L32)

L35 17804 SEA ABB=ON PLU=ON TANAKA S?/AU

L36 5183 SEA ABB=ON PLU=ON FUKUDA K?/AU

L37 998 SEA ABB=ON PLU=ON ASADA T?/AU

L38 1 SEA ABB=ON PLU=ON L35 AND L36 AND L37

L39 41 SEA ABB=ON PLU=ON L35 AND (L36 OR L37)

L40 1 SEA ABB=ON PLU=ON L36 AND L37

L41 85 SEA ABB=ON PLU=ON (L35 OR L36 OR L37) AND L32

L42 1 SEA ABB=ON PLU=ON L38 OR L40

L43 11 SEA ABB=ON PLU=ON L39 AND L32

FILE 'HCAPLUS' ENTERED AT 16:55:21 ON 26 MAR 2008

L44 17 SEA ABB=ON PLU=ON L27

L45 96 SEA ABB=ON PLU=ON L24

L46 1 SEA ABB=ON PLU=ON L45 AND (L35 OR L36 OR L37)

SEL AN

FILE 'MARPAT' ENTERED AT 16:55:57 ON 26 MAR 2008

L47 1 SEA ABB=ON PLU=ON ("140:321236"/AN OR "2004:292019"/AN)

L48 1 SEA ABB=ON PLU=ON L47 AND L27

FILE 'REGISTRY' ENTERED AT 16:56:29 ON 26 MAR 2008

FILE 'ZCAPLUS' ENTERED AT 16:56:32 ON 26 MAR 2008

D STAT QUE L38

D STAT QUE L43

FILE 'WPIX' ENTERED AT 16:56:54 ON 26 MAR 2008

L49 10 SEA ABB=ON PLU=ON L39 AND L32

FILE 'STNGUIDE' ENTERED AT 16:57:04 ON 26 MAR 2008

FILE 'ZCAPLUS, WPIX' ENTERED AT 16:57:13 ON 26 MAR 2008

L50 41 DUP REM L38 L39 L49 (11 DUPLICATES REMOVED)

ANSWERS '1-41' FROM FILE ZCAPLUS

L51 11 DUP REM L38 L43 L49 (11 DUPLICATES REMOVED)

ANSWERS '1-11' FROM FILE ZCAPLUS

D IBIB ABS HITIND HITSTR L51 1-11

FILE 'MARPAT' ENTERED AT 16:58:25 ON 26 MAR 2008

D STAT QUE L48

D IBIB ABS QHIT 1 L48

FILE 'REGISTRY' ENTERED AT 16:58:53 ON 26 MAR 2008

FILE 'ZCAPLUS' ENTERED AT 16:58:56 ON 26 MAR 2008

D STAT QUE L14

D STAT QUE L15

D STAT QUE L16

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D STAT QUE L33
D STAT QUE L34
L52 7 SEA ABB=ON PLU=ON (L14 OR L15 OR L16) OR (L33 OR L34)
L53 6 SEA ABB=ON PLU=ON L52 NOT (L38 OR L43)

FILE 'BEILSTEIN' ENTERED AT 16:59:48 ON 26 MAR 2008
D STAT QUE L21

FILE 'MARPAT' ENTERED AT 17:00:01 ON 26 MAR 2008
D STAT QUE L27
L54 16 SEA ABB=ON PLU=ON L27 NOT L48

FILE 'ZCAPLUS, BEILSTEIN, MARPAT' ENTERED AT 17:00:26 ON 26 MAR 2008
L55 26 DUP REM L53 L21 L54 (0 DUPLICATES REMOVED)
ANSWERS '1-6' FROM FILE ZCAPLUS
ANSWERS '7-10' FROM FILE BEILSTEIN
ANSWERS '11-26' FROM FILE MARPAT
D IBIB ABS HITIND HITSTR L55 1-6
D IDE ALLREF L55 7-10
D IBIB ABS QHIT L55 11-26

FILE HOME

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 25 MAR 2008 HIGHEST RN 1010115-69-1
DICTIONARY FILE UPDATES: 25 MAR 2008 HIGHEST RN 1010115-69-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

FILE ZCAPLUS

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FILE COVERS 1907 - 26 Mar 2008 VOL 148 ISS 13
FILE LAST UPDATED: 25 Mar 2008 (20080325/ED)

10/529290

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This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE BEILSTEIN

FILE LAST UPDATED ON January 3, 2008

FILE COVERS 1771 TO 2007.

FILE CONTAINS 10,119,480 SUBSTANCES

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For more detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. *
* FOR PRICE INFORMATION SEE HELP COST *

>>> Price change as of January 1st, 2008: Connect Time and Structure Search fees re-introduced. See NEWS and HELP COST <<<

FILE MARPAT

FILE CONTENT: 1961-PRESENT VOL 148 ISS 11 (20080321/ED)

SOME MARPAT RECORDS ARE DERIVED FROM INPI DATA FOR 1961-1987

MOST RECENT CITATIONS FOR PATENTS FROM MAJOR ISSUING AGENCIES (COVERAGE TO THESE DATES IS NOT COMPLETE):

US	2008032917	07	FEB	2008
DE	102006035202	31	JAN	2008
EP	1882693	30	JAN	2008
JP	2008024674	07	FEB	2008
WO	2008021152	21	FEB	2008
GB	2439172	19	DEC	2007
FR	2904316	01	FEB	2008
RU	2316552	10	FEB	2008
CA	2593150	06	JAN	2008

Expanded G-group definition display now available.

Effective December 15th the iteration and answer limits in MARPAT have increased from 100,000 to 200,000 for both on-line and batch searches. For more information on MARPAT search limits, type HELP SLIMITS at an arrow prompt.

FILE HCAPLUS

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FILE COVERS 1907 - 26 Mar 2008 VOL 148 ISS 13
FILE LAST UPDATED: 25 Mar 2008 (20080325/ED)

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FILE WPIX

FILE LAST UPDATED: 24 MAR 2008 <20080324/UP>
MOST RECENT THOMSON SCIENTIFIC UPDATE: 200820 <200820/DW>
DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

>>> IPC Reform backfile reclassification has been loaded to the end of November 2007. No update date (UP) has been created for the reclassified documents, but they can be identified by 20060101/UPIC and 20061231/UPIC, 20070601/UPIC, 20071001/UPIC and 20071130/UPIC. <<<

FOR A COPY OF THE DERWENT WORLD PATENTS INDEX STN USER GUIDE, PLEASE VISIT:
http://www.stn-international.de/training_center/patents/stn_guide.pdf

FOR DETAILS OF THE PATENTS COVERED IN CURRENT UPDATES, SEE
<http://scientific.thomson.com/support/patents/coverage/latestupdates/>

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http://www.stn-international.com/archive/presentations/DWPIAnaVist2_0710.p

>>> XML document distribution format now available - See HELP XMLDOC <<<

>>> ECLA Codes and Current US National Classifications have been added - see NEWS and HELP CHANGE <<<

>>> HELP for European Patent Classifications see HELP ECLA, HELP ICO <<<

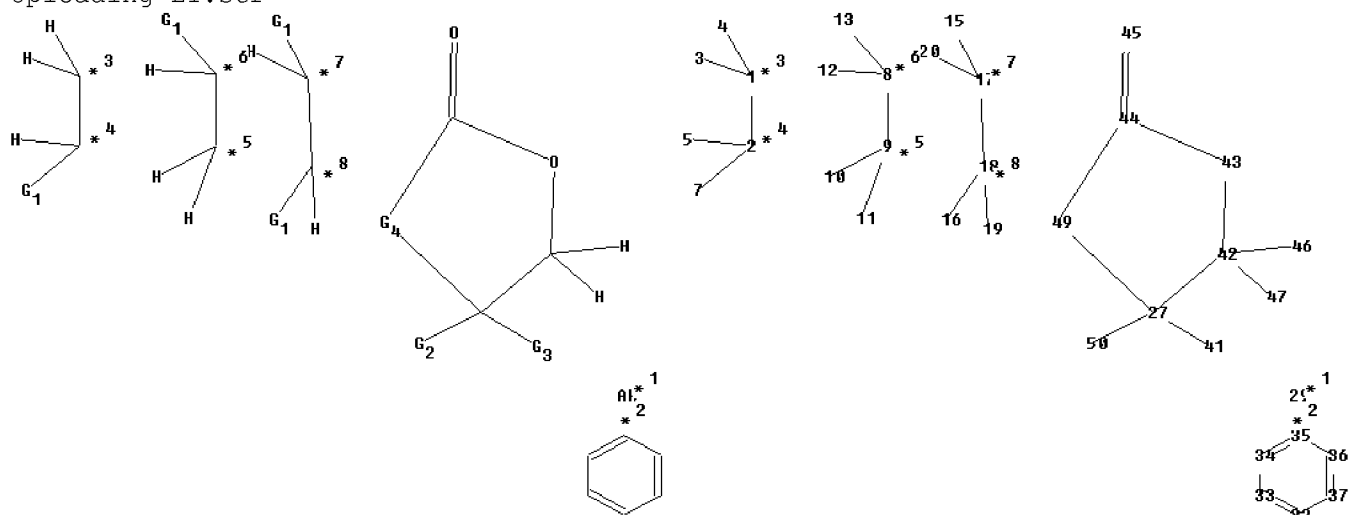
>>> Updated PDF files in the following links:
http://www.stn-international.de/stndatabases/details/ico_0801.zip
http://www.stn-international.de/stndatabases/details/epc_0801.zip
Supplement of all changed ECLA items:
http://www.stn-international.de/stndatabases/details/ecla_0802s.zip <<

FILE STNGUIDE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Mar 21, 2008 (20080321/UP).

10/529290

Uploading L1.str



```

chain nodes :
3 4 5 7 10 11 12 13 15 16 19 20 29 41 45 46 47 50
ring nodes :
1 2 8 9 17 18 27 32 33 34 35 36 37 42 43 44 49
chain bonds :
1-3 1-4 2-5 2-7 8-12 8-13 9-10 9-11 15-17 16-18 17-20 18-19 27-41 27-50
42-46 42-47 44-45
ring bonds :
1-2 8-9 17-18 27-49 27-42 32-33 32-37 33-34 34-35 35-36 36-37 42-43 43-44
44-49
exact/norm bonds :
1-3 1-4 2-5 2-7 8-12 8-13 9-10 9-11 15-17 16-18 17-20 18-19 27-41 27-50
42-46 42-47 44-45
exact bonds :
1-2 8-9 17-18 27-49 27-42 42-43 43-44 44-49
normalized bonds :
32-33 32-37 33-34 34-35 35-36 36-37

```

G1:CH3,Et

G2:CH3,H

G3:[*1],[*2]

G4:[*3-*4],[*5-*6],[*7-*8]

Connectivity :

29:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:CLASS 4:CLASS 5:CLASS 7:CLASS 8:Atom 9:Atom 10:CLASS
11:CLASS

12:CLASS 13:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:CLASS 20:CLASS

27:Atom 29:CLASS

32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 41:CLASS 42:Atom 43:Atom

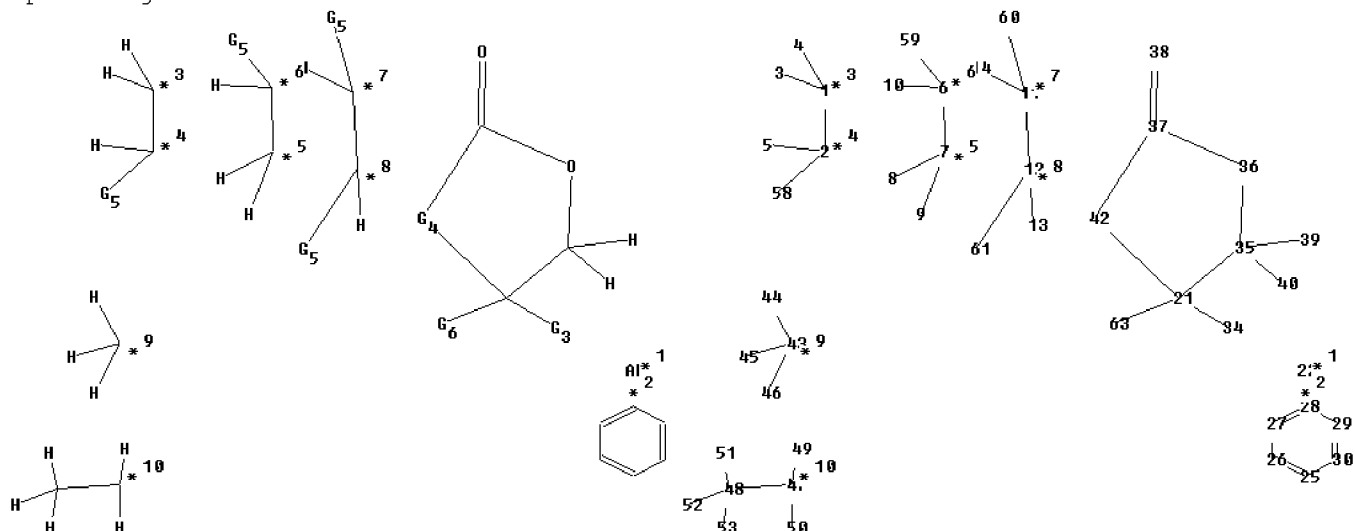
44:Atom 45:CLASS

46:CLASS 47:CLASS 49:Atom 50:CLASS

10/529290

Element Count :
Node 29: Limited
C,C3

Uploading L25.str



chain nodes :

3 4 5 8 9 10 13 14 22 34 38 39 40 43 44 45 46 47 48 49 50 51
52 53 58 59 60 61 63

ring nodes :

1 2 6 7 11 12 21 25 26 27 28 29 30 35 36 37 42

chain bonds :

1-3 1-4 2-5 2-58 6-10 6-59 7-8 7-9 11-14 11-60 12-13 12-61 21-34 21-63
35-39 35-40 37-38 43-44 43-45 43-46 47-48 47-49 47-50 48-51 48-52 48-53

ring bonds :

1-2 6-7 11-12 21-42 21-35 25-26 25-30 26-27 27-28 28-29 29-30 35-36 36-37
37-42

exact/norm bonds :

1-3 1-4 2-5 2-58 6-10 6-59 7-8 7-9 11-14 11-60 12-13 12-61 21-34 21-63
35-39 35-40 37-38 43-44 43-45 43-46 47-48 47-49 47-50 48-51 48-52 48-53

exact bonds :

1-2 6-7 11-12 21-42 21-35 35-36 36-37 37-42

normalized bonds :

25-26 25-30 26-27 27-28 28-29 29-30

G3:[*1],[*2]

G4:[*3-*4],[*5-*6],[*7-*8]

G5:[*9],[*10]

G6:H,[*9]

Connectivity :

22:1 E exact RC ring/chain

10/529290

Match level :

1:Atom 2:Atom 3:CLASS 4:CLASS 5:CLASS 6:Atom 7:Atom 8:CLASS 9:CLASS

10:CLASS

11:Atom 12:Atom 13:CLASS 14:CLASS 21:Atom 22:Atom 25:Atom 26:Atom 27:Atom

28:Atom 29:Atom

30:Atom 34:CLASS 35:Atom 36:Atom 37:Atom 38:Atom 39:CLASS 40:CLASS 42:Atom

43:Atom

44:CLASS 45:CLASS 46:CLASS 47:Atom 48:Atom 49:CLASS 50:CLASS 51:CLASS

52:CLASS 53:CLASS

58:CLASS 59:CLASS 60:CLASS 61:CLASS 63:CLASS

Element Count :

Node 22: Limited

C,C3